QUANTUM MECHANICS III

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CHAPTER OVERVIEW

1: Scattering Theory

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Thumbnail: Collimated homogeneous beam of monoenergetic particles, long wavepacket which is approximately a planewave, but strictly does not extend to infinity in all directions, is incident on a target and subsequently scattered into the detector subtending a solid angle. The detector is assumed to be far away from the scattering center. (Department of Physics Wiki @ Florida State University).

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1.1: Scattering Experiments on Quantum Particles

Quantum particles exhibit a feature known as **wave-particle duality**, which can be summarized in the **quantum double-slit thought experiment**. As shown in the figure below, a source emits electrons with energy E, which travel towards a screen with a pair of slits. A detector is positioned on the other side of the screen. By moving the detector around, we can measure the rate at which electrons are detected at different positions.

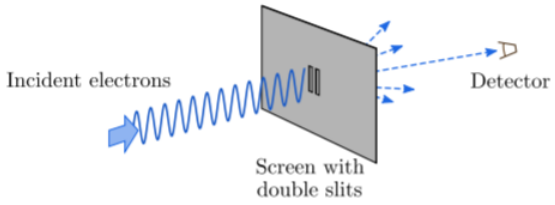

Figure 1.1.1

According to quantum theory, the experiment reveals the following: (i) the electrons arrive in discrete units—one at a time, like classical particles; (ii) when we move the detector around to measure how the detection events are *statistically* distributed in space, the resulting distribution matches an interference pattern formed by a classical wave diffracted by the slits. The wavelength λ is related to the electron energy E by

$$\lambda = \frac{2\pi}{k}, \quad E = \frac{\hbar^2 k^2}{2m}, \tag{1.1.1}$$

where $\hbar = h/2\pi$ is Dirac's constant, and m is the electron mass. (This also implies that we can deduce the spacing of the slits from the diffraction pattern, if E is known.)

Wave-particle duality arises from quantum theory's distinction between a particle's state and the outcomes of measurements performed on it. The state is described by a wavefunction $\psi(\mathbf{r})$, which can undergo diffraction like a classical wave. Measurement outcomes, however, depend *probabilistically* on the wavefunction. In a position measurement, the probability of locating a particle in a volume dV around position $\mathbf{r}$ is $|\psi(\mathbf{r})|^2\, dV$.

In this chapter, we will study a generalization of the double-slit experiment called a **scattering experiment**. The idea is to take an object called a **scatterer**, shoot quantum particles at it, and measure the resulting particle distribution. Just as the double-slit interference pattern can be used to deduce the slit spacing, a scattering experiment can be used to deduce various facts about the scatterer. Scattering experiments constitute a large proportion of the methods used to probe the quantum world—from electron- and photon-based laboratory experiments for measuring the properties of materials, to huge accelerator experiments that study high-energy phenomena like the Higgs boson.

We will focus on a simple scenario with a single non-relativistic quantum particle and a classical scatterer. Consider a continuous and unbounded d-dimensional space, describable by coordinates $\mathbf{r}$. Somewhere around the origin, $\mathbf{r} = 0$, is a finite-sized scatterer. An incoming quantum particle, with energy E, is governed by the Hamiltonian

$$\hat{H} = \hat{H}_0 + V(\hat{\mathbf{r}}), \quad \hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m}. \tag{1.1.2}$$

Here, $\hat{H}_0$ describes the particle's kinetic energy, m is the particle's mass, $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are position and momentum operators, and V is a **scattering potential** describing how the scatterer affects the quantum particle. We assume that $V(\mathbf{r}) \to 0$ as $|\mathbf{r}| \to \infty$, i.e., the scattering potential becomes negligible far from the origin.

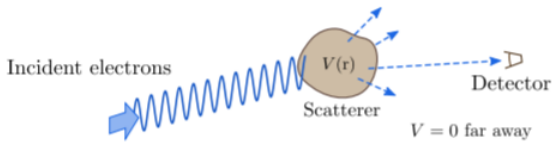

Figure 1.1.2

We prepare an incoming particle state with energy E, and want to see how the particle is scattered by the potential. However, converting these words into a well-defined mathematical problem is a bit tricky! We will give the formulation first, before

discussing its meaning:

1. The particle state $|\psi\rangle$ obeys the time-independent Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{1.1.3}$$

   where E is the incoming particle energy.

2. This state can be decomposed into two terms,

$$|\psi\rangle \; = \; |\psi_i\rangle + |\psi_s\rangle, \tag{1.1.4}$$

   where $|\psi_i\rangle$ is called the **incident state** and $|\psi_s\rangle$ is called the **scattered state**.

3. The incident state is described by a plane wave—a simultaneous eigenstate of $\hat{H}_0$ (with energy E) and $\hat{\mathbf{p}}$ (with momentum $\mathbf{p}_i$):

$$\hat{H}_0|\psi_i\rangle = E|\psi_i\rangle \;\text{ and }\; \hat{\mathbf{p}}|\psi_i\rangle = \mathbf{p}_i|\psi_i\rangle, \;\text{ where }\; E = \frac{|\mathbf{p}_i|^2}{2m}. \tag{1.1.5}$$

4. We require the scattered state to be an "outgoing" state. This is the most subtle of the conditions, and we will describe what it means later.

The first condition says that the scattering process is elastic. Since the scatterer takes the form of a potential $V(\mathbf{r})$, its interaction with the particle is conservative (i.e., the total energy E is fixed). The second condition says that the particle's wavefunction, $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$, consists of a superposition of an incoming wave and a scattered wave. The third condition defines the incoming wave as a plane wave whose wavelength is determined by the chosen energy E. The final condition says that the scattered wave moves out toward infinity.

Note that *this is not an eigenproblem*! Usually, when we use the time-independent Schrödinger equation, we treat it as an eigenproblem and solve for the energy eigenvalues and eigenstates. But in this case, E is an input to the calculation, describing the energy assigned to the incoming quantum particle. Given $|\psi_i\rangle$, E, and $V(\mathbf{r})$, we want to find $|\psi_s\rangle$.

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1.2: Recap- Position and Momentum States

Before proceeding, let us review the properties of quantum particles in free space. In a d-dimensional space, a coordinate vector $\mathbf{r}$ is a real vector of d components. A quantum particle can be described by the position basis—a set of quantum states $\{|\mathbf{r}\rangle\}$, one for each possible $\mathbf{r}$. If we are studying a particle trapped in a finite region (e.g., a particle in a box), $\mathbf{r}$ is restricted to that region; otherwise, $\mathbf{r}$ is any real d-dimensional vector. In either case, the $\mathbf{r}$'s are continuous, so the position eigenstates form an uncountably infinite set.

The position eigenstates are assumed to span the state space, so the identity operator can be resolved as

$$\hat{I} = \int d^d r \, |\mathbf{r}\rangle \, \langle \mathbf{r}|, \tag{1.2.1}$$

where the integral is taken over all allowed $\mathbf{r}$. It follows that

$$\langle \mathbf{r}|\mathbf{r}'\rangle = \delta^d(\mathbf{r}-\mathbf{r}'). \tag{1.2.2}$$

The position eigenstates are thus said to be "delta-function normalized", rather than being normalized to unity. In the above equation, $\delta^d(\cdots)$ denotes the d-dimensional delta function; for example, in 2D,

$$\langle x, y \,|\, x', y'\rangle = \delta(x-x')\,\delta(y-y'). \tag{1.2.3}$$

The position operator $\hat{\mathbf{r}}$ is defined by taking $|\mathbf{r}\rangle$ and $\mathbf{r}$ as its eigenstates and eigenvalues:

$$\hat{\mathbf{r}}|\mathbf{r}\rangle \; = \; \mathbf{r}\,|\mathbf{r}\rangle. \tag{1.2.4}$$

Momentum eigenstates are constructed from position eigenstates via Fourier transforms. First, suppose the allowed region of space is a box of length L on each side, with periodic boundary conditions in every direction. Define the set of wave-vectors $\mathbf{k}$ corresponding to plane waves satisfying the periodic boundary conditions at the box boundaries:

$$\left\{ \mathbf{k} \;\middle|\; k_j = 2\pi m/L \;\text{ for } m \in \mathbb{Z},\; j = 1, \ldots, d \right\}.$$

So long as L is finite, the $\mathbf{k}$ vectors are discrete. Now define

$$|\mathbf{k}\rangle = \frac{1}{L^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.2.5}$$

where the integral is taken over the box. These can be shown to satisfy

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k},\mathbf{k}'}, \quad \langle \mathbf{r}|\mathbf{k}'\rangle = \frac{1}{L^{d/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad I = \sum_{\mathbf{k}} |\mathbf{k}\rangle \, \langle \mathbf{k}|. \tag{1.2.6}$$

The momentum operator is defined so that its eigenstates are $\{|\mathbf{k}\rangle\}$, with $\hbar\mathbf{k}$ as the corresponding eigenvalues:

$$\hat{\mathbf{p}}|\mathbf{k}\rangle \; = \; \hbar\mathbf{k}\,|\mathbf{k}\rangle. \tag{1.2.7}$$

Thus, for finite L, the momentum eigenstates are discrete and normalizable to unity. The momentum component in each direction is quantized to a multiple of $\Delta p = 2\pi\hbar/L$.

We then take the limit of an infinite box, $L \to \infty$. In this limit, $\Delta p \to 0$, so the momentum eigenvalues coalesce into a continuum. It is convenient to re-normalize the momentum eigenstates by taking

$$|\mathbf{k}\rangle \to \left(\frac{L}{2\pi}\right)^{d/2} |\mathbf{k}\rangle. \tag{1.2.8}$$

In the $L \to \infty$ limit, the re-normalized momentum eigenstates satisfy

Definition: Re-normalized momentum eigenstates

$$|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.2.9}$$

$$|\mathbf{r}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d k \; e^{-i\mathbf{k}\cdot\mathbf{r}} |\mathbf{k}\rangle, \tag{1.2.10}$$

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta^d(\mathbf{k}-\mathbf{k}'), \quad \langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad I = \int d^d k \; |\mathbf{k}\rangle \, \langle \mathbf{k}|. \tag{1.2.11}$$

The above integrals are taken over infinite space, and the position and momentum eigenstates are now on a similar footing: both are delta-function normalized. In deriving the above equations, it is helpful to use the formula

$$\int_{-\infty}^{\infty} dx \;\; \exp(ikx) \;\; = \;\; 2\pi \, \delta(k). \tag{1.2.12}$$

For an arbitrary quantum state $|\psi\rangle$, a wavefunction is defined as the projection onto the position basis: $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$. Using the momentum eigenstates, we can show that

$$\begin{aligned} \langle \mathbf{r}|\hat{\mathbf{p}}|\psi\rangle &= \int d^d k \; \langle \mathbf{r}|\mathbf{k}\rangle \; \hbar\mathbf{k} \; \langle \mathbf{k}|\psi\rangle \\ &= \int \frac{d^d k}{(2\pi)^{d/2}} \; \hbar\mathbf{k} \; e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle \\ &= -i\hbar\nabla \int \frac{d^d k}{(2\pi)^{d/2}} \;\; e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle \\ &= -i\hbar\nabla\psi(\mathbf{r}). \end{aligned} \tag{1.2.13}$$

This result can also be used to prove Heisenberg's commutation relation $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

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1.3: Scattering From a 1D Delta-Function Potential

We are now ready to solve a simple scattering problem. Consider a 1D space with spatial coordinate denoted by x, and a scattering potential that consists of a "spike" at $x = 0$:

$$V(x) = \frac{\hbar^2 \gamma}{2m}\,\delta(x). \tag{1.3.1}$$

The form of the prefactor $\hbar^2\gamma/2m$ is chosen for later convenience; the parameter γ, which has units of $[1/x]$, controls the strength of the scattering potential.

Figure 1.3.1

If you are disturbed by the idea of a delta function potential, just regard it as the limiting case of a family of increasingly tall and narrow gaussian functions centered at $x = 0$. For each non-singular potential, the applicability of the Schrödinger wave equation implies that the wavefunction $\psi(x)$ is continuous and has well-defined first and second derivatives. In the delta function limit, however, these conditions are relaxed: $\psi(x)$ remains continuous, but at $x = 0$ the first derivative becomes discontinuous and the second derivative blows up. To see this, we integrate the Schrödinger wave equation over an infinitesimal range around $x = 0$:

$$\begin{aligned}\lim_{\varepsilon\to 0^+}\int_{-\varepsilon}^{+\varepsilon} dx\,\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar^2\gamma}{2m}\delta(x)\right]\psi(x) &= \lim_{\varepsilon\to 0^+}\int_{-\varepsilon}^{+\varepsilon} dx\; E\psi(x) \\ = \lim_{\varepsilon\to 0^+}\left\{-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{+\varepsilon}\right\} + \frac{\hbar^2\gamma}{2m}\psi(0) &= 0\end{aligned} \tag{1.3.2}$$

Hence,

$$\lim_{\varepsilon\to 0^+}\left\{\left.\frac{d\psi}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{x=-\varepsilon}\right\} = \gamma\,\psi(0). \tag{1.3.3}$$

To proceed, consider a particle incident from the left, with energy E. This is described by an incident state proportional to a momentum eigenstate $|k\rangle$, where $k = \sqrt{2mE/\hbar^2} > 0$. We said "proportional", not "equal", for it is conventional to adopt the normalization

$$|\psi_i\rangle = \sqrt{2\pi}\Psi_i|k\rangle \quad \Leftrightarrow \quad \psi_i(x) = \langle x|\psi\rangle = \Psi_i\, e^{ikx}. \tag{1.3.4}$$

The complex constant Ψ_i is called the "incident amplitude." Plugging this into the Schrödinger wave equation gives

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar^2\gamma}{2m}\delta(x)\right]\left(\Psi_i\, e^{ikx} + \psi_s(x)\right) = E\left(\Psi_i\, e^{ikx} + \psi_s(x)\right). \tag{1.3.5}$$

Taking $E = \hbar^2k^2/2m$, and doing a bit of algebra, simplifies this to

$$\left[\frac{d^2}{dx^2} + k^2\right]\psi_s(x) = \gamma\delta(x)\left(\Psi_i\, e^{ikx} + \psi_s(x)\right), \tag{1.3.6}$$

which is an inhomogenous ordinary differential equation for $\psi_s(x)$, with the potential on the right hand side acting as a "driving term".

To find the solution, consider the two regions $x < 0$ and $x > 0$. Since $\delta(x) \to 0$ for $x \neq 0$, the equation in each half-space reduces to

$$\left[\frac{d^2}{dx^2} + k^2\right]\psi_s(x) = 0. \tag{1.3.7}$$

This is the **Helmholtz equation**, whose general solution may be written as

$$\psi_s(x) = \Psi_i \left(f_1 \, e^{ikx} + f_2 \, e^{-ikx} \right). \tag{1.3.8}$$

Here, f_1 and f_2 are complex numbers that can take on different values in the two different regions $x < 0$ and $x > 0$.

We want $\psi_s(x)$ to describe an **outgoing wave**, moving away from the scatterer towards infinity. So it should be purely left-moving for $x < 0$, and purely right-moving for $x > 0$. To achieve this, let $f_1 = 0$ for $x < 0$, and $f_2 = 0$ for $x > 0$, so that $\psi_s(x)$ has the form

$$\psi_s(x) = \Psi_i \times \begin{cases} f_- \, e^{-ikx}, & x < 0 \\ f_+ \, e^{ikx}, & x > 0. \end{cases} \tag{1.3.9}$$

The complex numbers f_- and f_+ are called **scattering amplitudes**. They describe the magnitude and phase of the wavefunction scattered backwards into the $x < 0$ region, and scattered forward into the $x > 0$ region, respectively.

Recall from the discussion at the beginning of this section that $\psi(x)$ must be continuous everywhere, including at $x = 0$. Since $\psi_i(x)$ is continuous, $\psi_s(x)$ must be as well, so $f_- = f_+$. Moreover, we showed in Equation (1.3.3) that the first derivative of $\psi(x)$ is discontinuous at the scatterer. Plugging (1.3.3) into our expression for $\psi(x)$, at $x = 0$, gives

$$\Psi_i \left[ik(1 + f_\pm) - ik(1 - f_\pm) \right] = \Psi(1 + f_\pm)\gamma. \tag{1.3.10}$$

Hence, we obtain

$$f_+ = f_- = -\frac{\gamma}{\gamma - 2ik}. \tag{1.3.11}$$

For now, let us focus on the magnitude of the scattering amplitude (in the next chapter, we will see that the phase also contains useful information). The quantity $|f_\pm|^2$ describes the overall strength of the scattering process:

$$|f_\pm|^2 = \left[1 + \frac{8mE}{(\hbar\gamma)^2} \right]^{-1}. \tag{1.3.12}$$

Its dependence on E is plotted below:

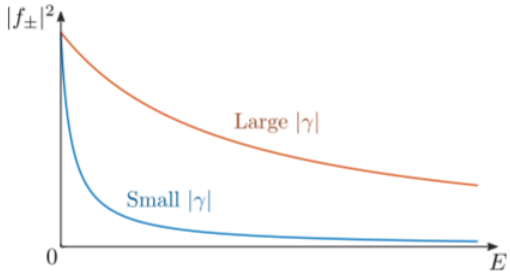

Figure 1.3.2

There are several notable features in this plot. First, for fixed potential strength γ, the scattering strength decreases monotonically with E—i.e., higher-energy particles are scattered less easily. Second, for given E, the scattering strength increases with $|\gamma|$, with the limit $|f|^2 \to 1$ as $|\gamma| \to \infty$. Third, an attractive potential ($\gamma < 0$) and a repulsive potential ($\gamma > 0$) are equally effective at scattering the particle.

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1.4: Scattering in 2D and 3D

We now wish to consider scattering experiments in spatial dimension $d \geq 2$, which have a new and important feature. For $d = 1$, the particle can only scatter forward or backward, but for $d \geq 2$ it can be scattered to the side.

Far from the scatterer, where $V(\mathbf{r}) \to 0$, the scattered wavefunction $\psi_s(\mathbf{r})$ satisfies

$$-\frac{\hbar^2}{2m}\nabla^2\psi_s(\mathbf{r}) = E\psi_s(\mathbf{r}), \tag{1.4.1}$$

where ∇^2 denotes the d-dimensional Laplacian. Let $E = \hbar^2 k^2/2m$, where $k \in \mathbf{R}^+$ is the wave-number in free space. Then the above equation can be written as

$$\left[\nabla^2 + k^2\right]\psi_s(\mathbf{r}) = 0, \tag{1.4.2}$$

which is the **Helmholtz equation** in d-dimensional space.

One set of elementary solutions to the Helmholtz equation are the plane waves

$$\left\{\exp(i\mathbf{k}\cdot\mathbf{r}), \quad \text{where} \quad |\mathbf{k}| = k\right\}. \tag{1.4.3}$$

But we're looking for an outgoing solution, and a plane wave can't be said to be "outgoing".

Therefore, we turn to curvilinear coordinates. In 2D, we use the polar coordinates (r, ϕ). We will skip the mathematical details of how to solve the 2D Helmholtz equation in these coordinates; the result is that the general solution can be written as a linear combination

$$\psi(\mathbf{r}) = \sum_{\pm}\sum_{m=-\infty}^{\infty} c_m^{\pm}\,\Psi_m^{\pm}(r,\phi), \quad \text{where} \quad \Psi_m^{\pm}(r,\phi) = H_m^{\pm}(kr)\,e^{im\phi}. \tag{1.4.4}$$

This is a superposition of circular waves $\Psi_m^{\pm}(r,\phi)$, with coefficients $c_m^{\pm} \in \mathbb{C}$. Each circular wave is a solution to the 2D Helmholtz equation with angular momentum quantum number $m \in \mathbb{Z}$. Its r-dependence is given by $H_m^{\pm}$, called a **Hankel function** of the "first kind" $(+)$ or "second kind" $(-)$. Some Hankel functions of the first kind are plotted below:

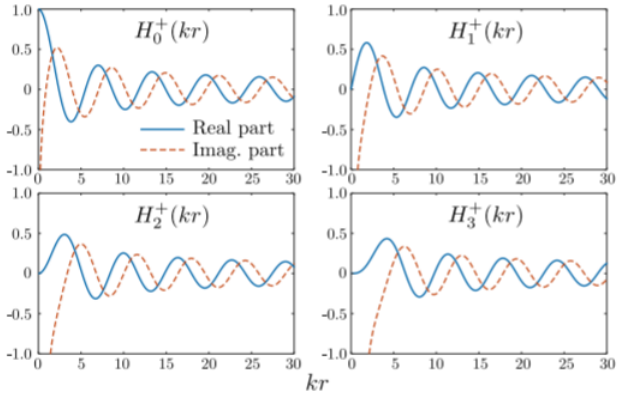

Figure 1.4.1

The H_m^- functions are the complex conjugates of H_m^+. For large values of the input,

$$H_m^{\pm}(kr) \overset{r\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi kr}}\,\exp\left[\pm i\left(kr - \frac{(m+\frac{1}{2})\pi}{2}\right)\right] \sim r^{-1/2}e^{\pm ikr}. \tag{1.4.5}$$

Therefore, the $\pm$ index specifies whether the circular wave is an **outgoing wave** directed outward from the origin $(+)$, or an **incoming wave** directed toward the origin $(-)$.

The 3D case is treated similarly. We use spherical coordinates (r, θ, ϕ), and the solutions of the 3D Helmholtz equation are superpositions of incoming and outgoing spherical waves:

$$\psi(\mathbf{r}) = \sum_{\pm} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{\ell m}^{\pm}\, \Psi_{\ell m}^{\pm}(r,\theta,\phi) \quad \text{where} \quad \Psi_{\ell m}^{\pm}(r,\theta,\phi) = h_{\ell}^{\pm}(kr)\, Y_{\ell m}(\theta,\phi). \tag{1.4.6}$$

The $c_{\ell m}^{\pm}$ factors are complex coefficients. Each $h_{\ell}^{\pm}$ is a **spherical Hankel function**, and each $Y_{\ell m}$ is a **spherical harmonic**. The ℓ and m indices specify the angular momentum of the spherical wave. For large inputs, the spherical Hankel functions have the limiting form

$$h_{\ell}^{\pm}(kr) \stackrel{r\to\infty}{\longrightarrow} \pm \frac{\exp\left[\pm i\left(kr - \frac{\ell\pi}{2}\right)\right]}{ikr}. \tag{1.4.7}$$

Hence, the $\pm$ index specifies whether the spherical wave is outgoing $(+)$ or incoming $(-)$. More discussion about these spherical waves can be found in Appendix A.

It is now clear what we need to do to get a scattered wavefunction $\psi_s(\mathbf{r})$ that is outgoing at infinity. We take a superposition with only outgoing $(+)$ wave components:

$$\psi_s(\mathbf{r}) = \begin{cases} \displaystyle\sum_m c_m^{+}\, H_m^{+}(kr)\, e^{im\phi}, & d = 2 \\ \displaystyle\sum_{\ell m} c_{\ell m}^{+}\, h_{\ell}^{+}(kr)\, Y_{\ell m}(\theta,\phi), & d = 3. \end{cases} \tag{1.4.8}$$

For large r, the outgoing wavefunction has the r-dependence

$$\psi_s(\mathbf{r}) \stackrel{r\to\infty}{\sim} r^{\frac{1-d}{2}}\, \exp(ikr). \tag{1.4.9}$$

For $d > 1$, the magnitude of the wavefunction decreases with distance from the origin. This is as expected, because with increasing r each outgoing wave spreads out over a wider area. The probability current density is $\mathbf{J} = (\hbar/m)\mathrm{Im}\left[\psi_s^* \nabla \psi_s\right]$, and its r-component is

$$\begin{aligned} J_r &\stackrel{r\to\infty}{\sim} \mathrm{Im}\left[r^{\frac{1-d}{2}}\, e^{-ikr}\, \frac{\partial}{\partial r}\left(r^{\frac{1-d}{2}}\, e^{ikr} \right) \right] \\ &= \mathrm{Im}\left[\frac{1-d}{2}\, r^{-d} + ikr^{1-d} \right] \\ &= k\, r^{1-d}. \end{aligned} \tag{1.4.10}$$

In d dimensions, the area of a wave-front scales as r^{d-1}, so the probability flux goes as $J_r\, r^{d-1} \sim k$, which is positive and independent of r. This describes a constant probability flux flowing outward from the origin. Note that if we plug $d = 1$ into the above formula, we find that J_r scales as r^0 (i.e., a constant), consistent with the results of the previous section: waves in 1D do not spread out with distance as there is no transverse dimension.

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1.5: The Scattering Amplitude and Scattering Cross Section

We can use the results of the previous section to systematically characterize the outcomes of a scattering experiment. Let the incident wavefunction be a plane wave,

$$\psi_i(\mathbf{r}) = \Psi_i\, e^{i\mathbf{k}_i\cdot\mathbf{r}}, \tag{1.5.1}$$

in d-dimensional space. Here, $\Psi_i \in \mathbb{C}$ is the **incident wave amplitude**, and $\mathbf{k}_i$ is the incident momentum. Let $k = |\mathbf{k}_i|$ denote its magnitude, so that the particle energy is $E = \hbar^2 k^2/2m$. We adopt coordinates (r, Ω), where r is the distance from the origin. For 1D, $\Omega \in \pm$ which specifies the choice of "forward" or "backward" scattering; for 2D polar coordinates, $\Omega = \phi$; and for 3D spherical coordinates, $\Omega = (\theta, \phi)$.

Far from the origin, the scattered wavefunction reduces to the form

$$\psi_s(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} \Psi_i\, r^{\frac{1-d}{2}}\, e^{ikr}\, f(\Omega). \tag{1.5.2}$$

The complex function $f(\Omega)$, called the **scattering amplitude**, is the fundamental quantity of interest in scattering experiments. It describes how the particle is scattered in various directions, depending on the inputs to the problem (i.e., $\mathbf{k}_i$ and the scattering potential).

Sometimes, we write the scattering amplitude using the alternative notation

$$f(\mathbf{k}_i \to \mathbf{k}_f), \quad \text{where } \mathbf{k}_f = k\hat{\mathbf{r}}. \tag{1.5.3}$$

This emphasizes firstly that the incident wave-vector is $\mathbf{k}_i$; and secondly that the particle is scattered in some direction which can be specified by either the unit position vector $\hat{\mathbf{r}}$, or equivalently by the momentum vector $\mathbf{k}_f = k\hat{\mathbf{r}}$, or by the angular coordinates Ω.

From the scattering amplitude, we define two other important quantities of interest:

Definition: Scattering Cross Sections

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2 \qquad (\text{the } \textbf{differential scattering cross section}) \tag{1.5.4}$$

$$\sigma = \int d\Omega\, |f(\Omega)|^2 \qquad (\text{the } \textbf{total scattering cross section}). \tag{1.5.5}$$

In the second equation, $\int d\Omega$ denotes the integral(s) over all the angle coordinates; for 1D, this is instead a discrete sum over the two possible directions, forward and backward.

The term "cross section" comes from an analogy with the scattering of classical particles. Consider the probablity current density associated with the scattered wavefunction:

$$\mathbf{J}_s = \frac{\hbar}{m}\mathrm{Im}\big[\psi_s^*\nabla\psi_s\big]. \tag{1.5.6}$$

Let us focus only on the r-component of the current density, in the $r\to\infty$ limit:

$$\begin{aligned} J_{s,r} &= \frac{\hbar}{m}\,\mathrm{Im}\left[\psi_s^*\frac{\partial}{\partial r}\psi_s\right] \\ &\overset{r\to\infty}{\longrightarrow} \frac{\hbar}{m}\,|\Psi_i|^2\,|f(\Omega)|^2\mathrm{Im}\left[\left(r^{\frac{1-d}{2}}\,e^{ikr}\right)^*\frac{\partial}{\partial r}\left(r^{\frac{1-d}{2}}\,e^{ikr}\right)\right] \\ &= \frac{\hbar k}{m}\,|\Psi_i|^2\,|f(\Omega)|^2\,r^{1-d}. \end{aligned} \tag{1.5.7}$$

The total flux of outgoing probability is obtained by integrating $J_{s,r}$ over a constant-r surface:

$$I_s = \int d\Omega\, r^{d-1}\, J_{s,r} = \frac{\hbar k}{m}\,|\Psi_i|^2\int d\Omega\,|f(\Omega)|^2. \tag{1.5.8}$$

We can assign a physical interpretation to each term in this result. The first factor, $\hbar k/m$, is the particle's speed (i.e., the group velocity of the de Broglie wave). The second factor, $|\Psi_i|^2$, is the probability density of the incident wave, which has units of $[x^{-d}]$ (i.e., inverse d-dimensional "volume"). The product of these two factors represents the **incident flux**,

$$J_i = \frac{\hbar k}{m} \, |\Psi_i|^2. \tag{1.5.9}$$

This has units of $[x^{1-d}t^{-1}]$ (i.e., rate per unit "area").

Let us re-imagine this incident flux J_i as a stream of classical particles, and the scatterer as a "hard-body" scatterer that only interacts with those particles striking it directly:

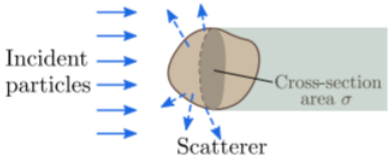

Figure 1.5.1

In this classical picture, the rate at which the incident particles strike the scatterer is

$$I_s = J_i \, \sigma, \tag{1.5.10}$$

where σ is the exposed cross-sectional area of the scatterer. Comparing this expression to Equation (1.5.8), we see that $\int d\Omega \, |f|^2$ plays a role analogous to the classical hard-body cross-sectional area. We hence call

$$\sigma \equiv \int d\Omega \, |f|^2 \tag{1.5.11}$$

the **total scattering cross section**. Moreover, the integrand $|f|^2$ is called the **differential scattering cross section**, for it represents the rate, per unit of solid angle, at which particles are scattered in a given direction. The total and differential scattering cross sections are the principal observable quantities that can be obtained from scattering experiments.

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1.6: The Green's Function

The scattering amplitude $f(\Omega)$ can be calculated using a variety of analytical and numerical methods. We will discuss one particularly important approach, based on a quantum variant of the Green's function technique for solving inhomogenous differential equations.

Let us return to the previously-discussed formulation of the scattering problem:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V} \\ \hat{H}|\psi\rangle &= E|\psi\rangle \\ |\psi\rangle &= |\psi_i\rangle + |\psi_s\rangle \\ \hat{H}_0|\psi_i\rangle &= E|\psi_i\rangle. \end{aligned} \tag{1.6.1}$$

These equations can be combined as follows:

$$\begin{aligned} \left(\hat{H}_0 + \hat{V}\right)|\psi_i\rangle + \hat{H}|\psi_s\rangle &= E\left(|\psi_i\rangle + |\psi_s\rangle\right) \\ \Rightarrow \quad \hat{V}|\psi_i\rangle + \hat{H}|\psi_s\rangle &= E|\psi_s\rangle \\ \Rightarrow \quad \left(E - \hat{H}\right)|\psi_s\rangle &= \hat{V}|\psi_i\rangle \end{aligned} \tag{1.6.2}$$

To proceed, we define the inverse of the operator on the left-hand side:

$$\hat{G} = \left(E - \hat{H}\right)^{-1}. \tag{1.6.3}$$

This operator is called the **Green's function**. Using it, we get

$$|\psi_s\rangle = \hat{G}\hat{V}|\psi_i\rangle. \tag{1.6.4}$$

Note that $\hat{G}$ depends on both the energy E and the scattering potential. To isolate the dependence on the scattering potential, let us define the Green's function for a free particle,

$$\hat{G}_0 = \left(E - \hat{H}_0\right)^{-1}. \tag{1.6.5}$$

This will be very useful for us, for $\hat{G}_0$ can be calculated exactly, whereas $\hat{G}$ often has no analytic expression. We can relate G and G_0 as follows:

$$\begin{aligned} \hat{G}(E - \hat{H}_0 - \hat{V}) &= I \quad \text{and} \quad (E - \hat{H}_0 - \hat{V})\hat{G} = I \\ \Rightarrow \quad \hat{G}\hat{G}_0^{-1} - \hat{G}\hat{V} &= I \quad \text{and} \quad \hat{G}_0^{-1}\hat{G} - \hat{V}\hat{G} = I. \end{aligned} \tag{1.6.6}$$

Upon respectively right-multiplying and left-multiplying these equations by $\hat{G}_0$, we arrive at the following pair of equations, called **Dyson's equations**:

Definition: Dyson's Equations

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}\hat{G}_0 \tag{1.6.7}$$

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G} \tag{1.6.8}$$

These equations are "implicit", as the unknown $\hat{G}$ appears in both the left and right sides.

Applying the second Dyson equation, Equation (1.6.8), to the scattering problem (1.6.4) gives

$$\begin{aligned} |\psi_s\rangle &= \left(\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}\right)\hat{V}|\psi_i\rangle \\ &= \hat{G}_0\hat{V}|\psi_i\rangle + \hat{G}_0\hat{V}\hat{G}\hat{V}|\psi_i\rangle \\ &= \hat{G}_0\hat{V}|\psi_i\rangle + \hat{G}_0\hat{V}|\psi_s\rangle \\ &= \hat{G}_0\hat{V}|\psi\rangle. \end{aligned} \tag{1.6.9}$$

This is a useful simplification, since it involves $\hat{G}_0$ rather than $\hat{G}$. The downside is that the equation is still implicit: the right-hand side involves the unknown total state $|\psi\rangle$, rather than the known incident state $|\psi_i\rangle$.

We can try to solve this implicit equation by using Equation (1.6.9) to get an expression for $|\psi\rangle$, then repeatedly plugging the result back into the right-hand side of Equation (1.6.9). This yields an infinite series formula:

$$\begin{aligned} |\psi_s\rangle &= \hat{G}_0\hat{V}\left(|\psi_i\rangle + \hat{G}_0\hat{V}|\psi\rangle\right) \\ &= \quad \vdots \\ &= \left[\hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle. \end{aligned} \tag{1.6.10}$$

Or, equivalently,

$$|\psi\rangle = \left[\hat{I} + \hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle. \tag{1.6.11}$$

This is called the **Born series**.

To understand its meaning, let us go to the position basis:

$$\begin{aligned} \psi(\mathbf{r}) = \psi_i(\mathbf{r}) &+ \int d^d r' \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\psi_i(\mathbf{r}') \\ &+ \int d^d r' d^d r'' \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\, \langle \mathbf{r}'|\hat{G}_0|\mathbf{r}''\rangle\, V(\mathbf{r}'')\psi_i(\mathbf{r}'') \\ &+ \cdots \end{aligned} \tag{1.6.12}$$

This formula can be regarded as a description of **multiple scattering**. Due to the presence of the scatterer, the particle wavefunction is a quantum superposition of terms describing zero, one, two, or more scattering events, as illustrated below:

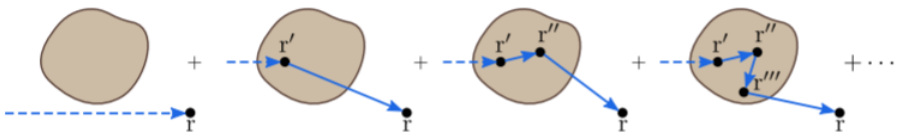

Figure 1.6.1

Each successive term in the Born series involves more scattering events, i.e., higher multiples of $\hat{V}$. For example, the second-order term is

$$\int d^d r' d^d r'' \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\, \langle \mathbf{r}'|\hat{G}_0|\mathbf{r}''\rangle\, V(\mathbf{r}'')\psi_i(\mathbf{r}''). \tag{1.6.13}$$

This describes the particle undergoing the following process: (i) scattering of the incident particle at point $\mathbf{r}''$, (ii) propagation from $\mathbf{r}''$ to $\mathbf{r}'$, (iii) scattering again at point $\mathbf{r}'$, and (iv) propagation from $\mathbf{r}'$ to $\mathbf{r}$. The scattering points $\mathbf{r}'$ and $\mathbf{r}''$ are integrated over, with all possible positions contributing to the result; since the integrals are weighted by V, those positions where the scattering potential are strongest will contribute the most.

For a sufficiently weak scatterer, it can be a good approximation to retain just the first few terms in the Born series. For the rest of this discussion, let us assume that such an approximation is valid. The question of what it means for $\hat{V}$ to be "sufficiently weak"—i.e., the exact requirements for the Born series to converge—is a complex topic beyond the scope of our present discussion.

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1.7: The Green's Function for a Free Particle

We have defined the free-particle Green's function as the operator $\hat{G}_0 = \left(E - \hat{H}_0\right)^{-1}$. Its representation in the position basis, $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$, is called the **propagator**. As we have just seen, when the Born series is written in the position basis, the propagator appears in the integrand and describes how the particle "propagates" between discrete scattering events.

The propagator is a solution to a partial differential equation:

$$\begin{aligned} \langle \mathbf{r}|\left(E - \hat{H}_0\right)\hat{G}_0|\mathbf{r}'\rangle &= \langle \mathbf{r}|\hat{I}\,|\mathbf{r}'\rangle \\ = \left(E + \frac{\hbar^2}{2m}\nabla^2\right)\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \delta^d(\mathbf{r}-\mathbf{r}') \\ \Rightarrow \qquad \left(\nabla^2 + k^2\right)\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \frac{2m}{\hbar^2}\delta^d(\mathbf{r}-\mathbf{r}'). \end{aligned} \tag{1.7.1}$$

As before, $k = \sqrt{2mE/\hbar^2}$ where E is the energy of the incident particle. Therefore, up to a factor of $2m/\hbar^2$, the propagator is the Green's function for the d-dimensional Helmholtz equation (see Section 1.4). Note that the ∇^2 acts upon the $\mathbf{r}$ coordinates, not $\mathbf{r}'$.

To solve for $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$, we can use the momentum eigenstates:

$$\begin{aligned} \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \langle \mathbf{r}|\hat{G}_0\left(\int d^d k'\,|\mathbf{k}'\rangle\langle\mathbf{k}'|\right)|\mathbf{r}'\rangle \\ &= \int d^d k'\ \langle \mathbf{r}|\mathbf{k}'\rangle\ \frac{1}{E - \frac{\hbar^2|\mathbf{k}'|^2}{2m}}\ \langle \mathbf{k}'|\mathbf{r}'\rangle \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^d}\int d^d k'\ \frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2 - |\mathbf{k}'|^2}. \end{aligned} \tag{1.7.2}$$

To proceed, we must specify the spatial dimension d. Let us set $d = 3$; the calculations for other d are fairly similar. To calculate the integral over the 3D wave-vector space, we adopt spherical coordinates (k', θ, ϕ), with the coordinate axes aligned so that $\mathbf{r} - \mathbf{r}'$ points along the $\theta = 0$ direction. We can now do the integral:

$$\begin{aligned} \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int d^3 k'\ \frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2 - |\mathbf{k}'|^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^\infty dk' \int_0^\pi d\theta \int_0^{2\pi} d\phi\ k'^2 \sin\theta\ \frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|\cos\theta)}{k^2 - k'^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk' \int_{-1}^1 d\mu\ k'^2\ \frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|\mu)}{k^2 - k'^2} \qquad (\text{letting } \mu = \cos\theta) \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk'\ \frac{k'^2}{k^2 - k'^2}\ \frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|) - \exp(-ik'|\mathbf{r}-\mathbf{r}'|)}{ik'|\mathbf{r}-\mathbf{r}'|} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\frac{i}{|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^\infty dk'\ \frac{k'\ \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k)(k'+k)} \end{aligned} \tag{1.7.3}$$

This looks like something we can handle with contour integration techniques. But there's a snag: the integration contour runs over the real-k' line, and since $k \in \mathbb{R}^+$, there are two poles on the contour (at $\pm k$). Hence, the value of the integral, as written, is singular.

To make the integral non-singular, we must "regularize" it by tweaking its definition. One way is to displace the poles infinitesimally in the complex k' plane, shifting them off the contour. We have a choice of whether to move each pole upwards or downwards; this choice turns out to be linked to whether the waves described by $\hat{G}_0$ are incoming, outgoing, or behave some other way at infinity. It turns out that the right choice for us is to move the pole at $-k$ infinitesimally downwards, and the pole at $+k$ infinitesimally upwards:

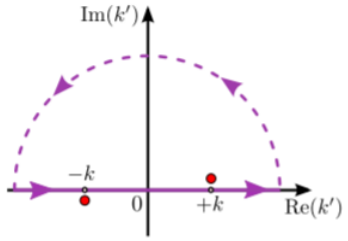

Figure 1.7.1

This means replacing the denominator of the integrand as follows:

$$(k'-k)(k'+k) \;\rightarrow\; (k'-k-i\varepsilon)(k'+k+i\varepsilon) = k'^2 - (k+i\varepsilon)^2, \tag{1.7.4}$$

where ε is a positive infinitesimal. This is equivalent to replacing $E \rightarrow E + i\varepsilon$ in the definition of the Green's function. The integral can now be computed as follows:

$$\begin{aligned}
\int_{-\infty}^{\infty} dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k)(k'+k)} &\rightarrow \lim_{\varepsilon\to 0^+} \int_{-\infty}^{\infty} dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)} \quad \text{(regularize)} \\
&= \lim_{\varepsilon\to 0^+} \int_{C} dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)} \quad \text{(close contour above)} \\
&= 2\pi i \lim_{\varepsilon\to 0^+} \operatorname{Res}\left[\frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)} \right]_{k'=k+i\varepsilon^+} \\
&= \pi i \exp(ik|\mathbf{r}-\mathbf{r}'|).
\end{aligned} \tag{1.7.5}$$

Plugging this into Equation (1.7.2) yields the propagator $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$. The final result is given below, along with the results for $d=1$ and $d=2$ (which are obtained in a similar fashion):

Definition: Propagator

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2} \times \begin{cases} \dfrac{1}{2ik}\exp(ik|x-x'|), & d=1 \\ \dfrac{1}{4i}H_0^+(k|\mathbf{r}-\mathbf{r}'|), & d=2 \\ -\dfrac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|}, & d=3. \end{cases} \tag{1.7.6}$$

The propagator can be regarded as a function of the position $\mathbf{r}$, describing a wave propagating outwards from a source point $\mathbf{r}'$. This outgoing behavior comes from our above choice of regularization, which tweaked the definition of the Green's function to be

Definition: Green's function

$$\hat{G}_0 = \lim_{\varepsilon\to 0^+} \left(E - \hat{H}_0 + i\varepsilon\right)^{-1}. \tag{1.7.7}$$

This is called an **outgoing** or **causal Green's function**. The word "causal" refers to the concept of "cause-and-effect": i.e., a source at one point of space (the "cause") leads to the emission of waves that move outwards (the "effect").

Different regularizations produce Green's functions with alternative features. For instance, we could flip the sign of $i\varepsilon$ in the Green's function redefinition, which displaces the k-space poles in the opposite direction. The resulting propagator $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$ is complex-conjugated, and describes a wave moving inwards from infinity, "sinking" into the point $\mathbf{r}'$. Such a choice of regularization thus corresponds to an **incoming Green's function**. In the scattering problem, we will always deal with the outgoing/causal Green's function.

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1.8: Scattering Amplitudes in 3D

The propagator can now be plugged into the scattering problem posed in Sections 1.5-1.6:

$$\begin{aligned} \psi_i(\mathbf{r}) &= \Psi_i\, e^{i\mathbf{k}\cdot\mathbf{r}}, \\ \psi_s(\mathbf{r}) &= \langle \mathbf{r}|\hat{G}_0\hat{V}|\psi\rangle \quad \overset{r\to\infty}{\longrightarrow} \quad \Psi_i\, r^{\frac{1-d}{2}}\, e^{ikr}\, f(\mathbf{k}_i \to k\hat{\mathbf{r}}). \end{aligned} \tag{1.8.1}$$

Our goal is to determine the scattering amplitude f. We will focus on the 3D case; the 1D and 2D cases are handled in a similar way.

In the $r \to \infty$ limit, the propagator can be simplified using the Taylor expansion

$$|\mathbf{r} - \mathbf{r}'| = r - \hat{\mathbf{r}}\cdot\mathbf{r}' + \cdots, \tag{1.8.2}$$

where $\hat{\mathbf{r}}$ denotes the unit vector pointing parallel to $\mathbf{r}$. (This is the same "large-r" expansion used in deriving the electric dipole moment in classical electromagnetism.) Applying this to the 3D outgoing propagator gives, to lowest order,

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle \overset{r\to\infty}{\approx} -\frac{2m}{\hbar^2}\,\frac{e^{ikr}}{4\pi r}\,\exp(-ik\,\hat{\mathbf{r}}\cdot\mathbf{r}') \tag{1.8.3}$$

Hence, the scattered wavefunction is

$$\begin{aligned} \psi_s(\mathbf{r}) &= \int d^3r'\, \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\,\psi(\mathbf{r}') \\ &\overset{r\to\infty}{\approx} -\frac{2m}{\hbar^2}\,\frac{e^{ikr}}{4\pi r}\int d^3r'\,\exp(-ik\,\hat{\mathbf{r}}\cdot\mathbf{r}')\,V(\mathbf{r}')\,\psi(\mathbf{r}') \\ &= -\frac{2m}{\hbar^2}\,\frac{e^{ikr}}{4\pi r}\,(2\pi)^{3/2}\,\langle \mathbf{k}_f|\hat{V}|\psi\rangle, \quad \text{where } \mathbf{k}_f \equiv k\hat{\mathbf{r}}. \end{aligned} \tag{1.8.4}$$

We can combine this with the Green's function relation from Section 1.6,

$$|\psi\rangle = \left(\hat{I} + \hat{G}\hat{V}\right)|\psi_i\rangle. \tag{1.8.5}$$

This yields

$$\begin{aligned} \psi_s(\mathbf{r}) &\overset{r\to\infty}{\longrightarrow} -\frac{2m}{\hbar^2}\,\frac{e^{ikr}}{r}\,\sqrt{\frac{\pi}{2}}\,\langle \mathbf{k}_f|\hat{V} + \hat{V}\hat{G}\hat{V}|\psi_i\rangle \\ &= -\frac{2m}{\hbar^2}\,\Psi_i\,\frac{e^{ikr}}{r}\,2\pi^2\,\langle \mathbf{k}_f|\hat{V} + \hat{V}\hat{G}\hat{V}|\mathbf{k}_i\rangle. \end{aligned} \tag{1.8.6}$$

This can be compared to the earlier definition of the scattering amplitude,

$$\psi_s(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} \Psi_i\frac{e^{ikr}}{r}f(\mathbf{k}_i \to \mathbf{k}_f). \tag{1.8.7}$$

Hence, we find that

Definition: Scattering

$$\begin{aligned} f(\mathbf{k}_i \to \mathbf{k}_f) &= -\frac{2m}{\hbar^2}\cdot 2\pi^2\,\langle \mathbf{k}_f|\hat{V} + \hat{V}\hat{G}\hat{V}|\mathbf{k}_i\rangle \\ &= -\frac{2m}{\hbar^2}\cdot 2\pi^2\,\langle \mathbf{k}_f|\hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \cdots|\mathbf{k}_i\rangle, \end{aligned} \tag{1.8.8}$$

subject to the elasticity constraint $|\mathbf{k}_i| = |\mathbf{k}_f|$. In deriving the last line, we used the Born series formula (1.6.11).

This result is the culmination of the numerous definitions and derivations from the preceding sections. On the left side is the scattering amplitude, the fundamental quantity of interest in scattering experiments. The right side contains quantities that are known to us, or that can be calculated: the initial and final momenta, the scattering potential, and the Green's function. Although

this result was derived for the 3D case, very similar formulas hold for other dimensions, but with the $2\pi^2$ factor replaced with other numerical factors.

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1.9: Example- Uniform Spherical Well in 3D

Let us test the Born series against a simple example, consisting of the scattering potential

$$V(\mathbf{r}) = \begin{cases} -U, & |\mathbf{r}| \le R \\ 0, & |\mathbf{r}| > 0. \end{cases} \tag{1.9.1}$$

We will assume that $U > 0$, so that the potential is attactive and describes a uniform spherically symmetric well of depth U and radius R, surrounded by empty space. For this potential, the scattering problem can be solved exactly, using the method of **partial wave analysis** described in Appendix A. The resulting scattering amplitudes are

$$\begin{aligned} f(\mathbf{k}_i \to \mathbf{k}_f) \;&= \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left(e^{2i\delta_\ell} - 1\right)\left(2\ell+1\right) P_\ell(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f), \\ \text{where} \;\; \delta_\ell \;&= \frac{\pi}{2} + \arg\left[k h_\ell^{+\prime}(kR)\, j_\ell(qR) - q h_\ell^{+}(kR)\, j_\ell'(qR)\right], \\ q &= \sqrt{2m(E+U)/\hbar^2} \\ k &\equiv |\mathbf{k}_i| = |\mathbf{k}_f|. \end{aligned} \tag{1.9.2}$$

This solution is expressed in terms of various special functions; j_ℓ and h_ℓ are the spherical Bessel function of the first kind and spherical Hankel function, while P_ℓ is the Legendre polynomial (which appears in the definition of the spherical harmonic functions).

We will pit this exact solution against the results from the Born series:

$$f(\mathbf{k}_i \to \mathbf{k}_f) \approx -\frac{2m}{\hbar^2} \cdot 2\pi^2 \left[\langle \mathbf{k}_f | \hat{V} | \mathbf{k}_i \rangle + \langle \mathbf{k}_f | \hat{V} \hat{G}_0 \hat{V} | \mathbf{k}_i \rangle + \cdots \right]. \tag{1.9.3}$$

The bra-kets can be evaluated in the position representation. Let us do this for just the first two terms in the series:

$$\begin{aligned} f(\mathbf{k}_i \to \mathbf{k}_f) &\approx -\frac{2m}{\hbar^2}\, 2\pi^2 \left[\int d^3 r_1 \, \frac{\exp(-i\mathbf{k}_f \cdot \mathbf{r}_1)}{(2\pi)^{3/2}} \, V(\mathbf{r}_1) \, \frac{\exp(i\mathbf{k}_i \cdot \mathbf{r}_1)}{(2\pi)^{3/2}} \right. \\ &\qquad \left. + \int d^3 r_1 \int d^3 r_2 \, \frac{\exp(-i\mathbf{k}_f \cdot \mathbf{r}_2)}{(2\pi)^{3/2}} \, V(\mathbf{r}_2) \, \langle \mathbf{r}_2 | \hat{G}_0 | \mathbf{r}_1 \rangle \, V(\mathbf{r}_1) \, \frac{\exp(i\mathbf{k}_i \cdot \mathbf{r}_1)}{(2\pi)^{3/2}} \right] \\ &= \frac{1}{4\pi} \left[\frac{2mU}{\hbar^2} \int_{|\mathbf{r}_1| \le R} d^3 r_1 \; \exp[i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}_1] \right. \\ &\qquad \left. + \left(\frac{2mU}{\hbar^2}\right)^2 \int_{|\mathbf{r}_1|<R} d^3 r_1 \int_{|\mathbf{r}_2|<R} d^3 r_2 \; \frac{\exp[i(k|\mathbf{r}_1 - \mathbf{r}_2| - \mathbf{k}_f \cdot \mathbf{r}_2 + \mathbf{k}_i \cdot \mathbf{r}_1)]}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|} \right]. \end{aligned} \tag{1.9.4}$$

If we use only the first term in the Born series, the result is called the “first Born approximation”; if we use two terms, the result is called the “second Born approximation”. Higher-order Born approximations can be derived in a similar fashion.

The most expedient way to calculate these integrals is to use Monte Carlo integration. To find an integral of the form

$$I = \int_{|\mathbf{r}|<R} d^3 r \, F(\mathbf{r}), \tag{1.9.5}$$

we randomly sample N points within a cube of volume $(2R)^3$ centered around the origin, enclosing the desired sphere of radius R. For the n-th sampled point, $\mathbf{r}_n$, we compute

$$F_n = \begin{cases} F(\mathbf{r}_n), & |\mathbf{r}| < R \\ 0, & \text{otherwise.} \end{cases} \tag{1.9.6}$$

The F_n’s give the values of the integrand at the sampling points, omitting the contribution from points outside the sphere. Then we estimate the integral as

$$I \approx (2R)^3 \langle F_n \rangle = \frac{(2R)^3}{N} \sum_{n=1}^{N} F_n. \tag{1.9.7}$$

The estimate converges to the true value as $N \to \infty$; in practice, $N \sim 10^4$ yields a good result for typical 3D integrals, and can be computed in around a second on a modern computer. Similarly, to calculate the double integral appearing in the second term of the Born series, we sample *pairs* of points; the volume factor $(2R)^3$ is then replaced by $(2R)^6$.

This method for calculating the Born series can be readily generalized to more complicated scattering potentials, including potentials for which there is no exact solution.

The figure below shows the results of the Born approximation for the uniform potential well, compared to the "exact" solution computed from partial wave analysis. It plots $|f|^2$ versus the scattering energy E, for the case of 90° scattering (i.e., $\mathbf{k}_f$ perpendicular to $\mathbf{k}_i$), with wells of different depth U and the same radius $R = 1$. We adopt computational units $\hbar = m = 1$, and each Monte Carlo integral is computed using 3×10^4 samples.

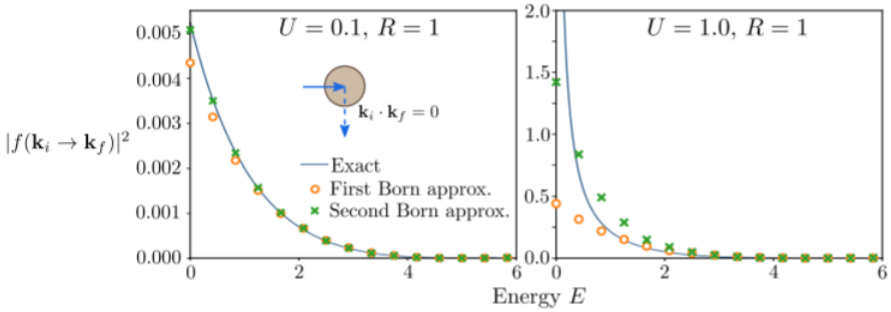

Figure 1.9.1

The first thing to notice in these results in that $|f|^2$ diminishes to zero for large E. This makes sense, since the scattering potential has some energy scale (U), so a incident particle that is too energetic ($E \gg U$) will just zoom through, with little chance of being deflected.

Looking more closely at the plots, we see that for the shallower well ($U = 0.1$), the first Born approximation agrees well with the exact results, and the second Born approximation is even better, particularly for small E. For the deeper well ($U = 1$), the Born approximations do not match the exact results. Roughly speaking, for the stronger scattering potential, an incident particle has a higher chance to undergo multiple-scattering (i.e., bouncing around the potential multiple times before escaping), which means that higher terms in the Born series become more important. In fact, if the potential is too strong, taking the Born approximation to higher orders might not even work, as the Born series itself can become non-convergent. In those cases, different methods must be brought to bear. We will see an example in the next chapter, in the form of phenomena known as "scattering resonances".

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1.10: Exercises

Exercises

Exercise 1.10.1

In Sec. 1.2, we derived the eigenstates of a particle in an empty infinite space by considering a box of length L on each side, applying periodic boundary conditions, and taking $L \to \infty$. Suppose we instead use Dirichlet boundary conditions (i.e., the wavefunction vanishes on the walls of the box). Show that this gives rise to the same set of momentum eigenstates in the $L \to \infty$ limit.

Exercise 1.10.2

Using the results for the 1D delta-function scattering problem described in Section 1.3, calculate the probability current

$$J(x) = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right), \tag{1.10.1}$$

where $\psi(x)$ is the *total* (incident + scattered) wavefunction. Explain the relationship between the values of J on the left and right side of the scatterer.

Exercise 1.10.3

Derive the Green's function for a free particle in 1D space:

$$\langle x|\hat{G}_0|x'\rangle = \frac{2m}{\hbar^2} \cdot \frac{1}{2ik_i}\exp(ik_i|x - x'|). \tag{1.10.2}$$

Exercise 1.10.4

In Section 1.8, the scattering amplitude $f(\mathrm{k} \to \mathrm{k}')$ for the 3D scattering problem was derived using the Born series. Derive the corresponding expressions for 1D and 2D.

Further Reading

[1] Bransden & Joachain, §13.1—13.3 and §13.5—13.6.

[2] Sakurai, §7.1–7.3, 7.5–7.6

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CHAPTER OVERVIEW

2: Resonances

2.1: Bound States and Free States
2.2: Quasi-Bound States and Resonances
2.3: Green's Function Analysis of Scattering Resonances
2.4: Fermi's Golden Rule
2.5: Fermi's Golden Rule in a 1D Resonance Model
2.6: Exercises

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2.1: Bound States and Free States

A curious feature of wavefunctions in infinite space is that they can have two distinct forms: (i) **bound states** that are localized to one region, and (ii) **free states** that extend over the whole space. Both kinds of states can co-exist in a single system. A simple model exhibiting this is the **1D finite square well**. Consider the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} - U\,\Theta(a - |\hat{x}|), \tag{2.1.1}$$

where $\hat{x}$ and $\hat{p}$ are 1D position and momentum operators, m is the particle mass, U and a are positive real parameters governing the potential function, and Θ denotes the Heaviside step function (1 if the input is positive, and 0 otherwise). As shown below, the potential forms a well of depth U and width $2a$. Outside the well, the potential is zero.

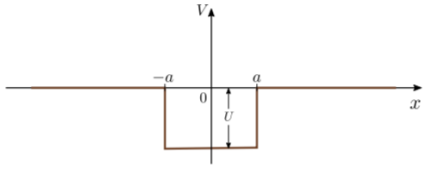

Figure 2.1.1

For such a Hamiltonian, the time-independent Schrödinger wave equation can be solved efficiently using a technique called the **transfer matrix method**. Here, we will describe a few key aspects of the calculation, bypassing most of the details. For a fuller discussion of the transfer matrix method, refer to Appendix B.

We begin by noting that obtaining solutions to the Schrödinger wave equation first requires specifying the boundary conditions at infinity. The choice of boundary conditions determines whether the solution we get is a bound state or free state.

For a bound state, we require the wavefunction to diminish exponentially as $x \to \pm\infty$. In the exterior region ($|x| > a$), the Schrödinger wave equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x), \tag{2.1.2}$$

subject to the boundary conditions

$$\psi(x) \overset{x\to\pm\infty}{\sim} e^{\mp\kappa x}, \quad \mathrm{Re}(\kappa) > 0. \tag{2.1.3}$$

Therefore, in the exterior region the bound state solutions take the form

$$\psi(x) = c_\pm\, e^{\mp\kappa x}, \quad \text{where} \quad -\frac{\hbar^2\kappa^2}{2m} = E, \quad c_\pm \in \mathbb{C}. \tag{2.1.4}$$

Given that E is real, it follows that κ is real, so $E < 0$. Moreover, the variational principle implies that $E \geq -U$, so bound state energies are restricted to the range $-U \leq E < 0$.

It is also possible to show that the bound state energies are *discrete*: the energy spacing decreases with a, but so long as a is finite, the spacing is non-vanishing. Furthermore, the wavefunction for a bound state can always be normalized:

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx \;=\; 1. \tag{2.1.5}$$

The normalization integral is finite since $|\psi(x)|^2$ vanishes exponentially for $x \to \pm\infty$. These properties follow from the analysis of the general class of "Sturm-Liouville-type" differential equations; for details, refer to textbooks such as Courant and Hilbert (1953).

For a free state, the situation is quite different. The wavefunction does not vanish exponentially at infinity, but takes the form

$$\psi(x) = \begin{cases} \alpha_-\, e^{ikx} + \beta_-\, e^{-ikx}, & x < -a \\ (\text{something}), & -a < x < a \\ \alpha_+\, e^{ikx} + \beta_+\, e^{-ikx}, & x > a. \end{cases} \tag{2.1.6}$$

Inside the potential well, $\psi(x)$ varies in some complicated way; on the outside, it consists of superpositions of left-moving and right-moving plane waves with real wavenumber k. The coefficients $\alpha_\pm$ and $\beta_\pm$ are not independent quantities, but are linked by a linear relation (see Appendix B). To satisfy Schrödinger's equation, we must have

$$\frac{\hbar^2 k^2}{2m} = E, \tag{2.1.7}$$

which implies that free states only occur for $E \geq 0$. These solutions form a continuum: there are free states for *every* $E \geq 0$. Since $|\psi(x)|^2$ does not diminish at infinity, the integral $\int_{-\infty}^{\infty} |\psi(x)|^2\, dx$ is divergent, so the wavefunctions have no finite normalization.

The following figure shows numerically-obtained results for a square well with $U = 30$ and $a = 1$ (in units where $\hbar = m = 1$). The energy spectrum is shown on the left side. There exist five bound states; their plots of $|\psi|^2$ versus x are shown on the right side. These results were computed using the transfer matrix method described in Appendix B.

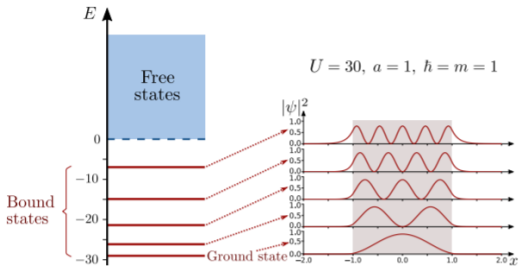

Figure 2.1.2

Many of the lessons drawn from the square well model can be generalized to more complicated potentials. In cases where the potential at infinity is V_{ext} rather than zero, free states occur for $E \geq V_{\text{ext}}$ and bound states occur for $\min(V) < E < V_{\text{ext}}$.

There is an important proviso to bear in mind. If we vary the potential, the number of bound states can change: i.e., bound state solutions can either appear or disappear. A numerical example is given below, showing the bound state energies for the square well model with fixed $a = 1$, as we vary the potential minimum $-U$:

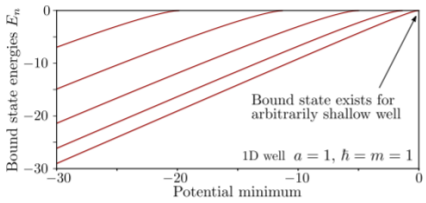

Figure 2.1.3

For $U = 30$, there are five bound states, which disappear one by one as we make the potential well shallower. Note that one bound state survives in the limit $U \to 0$. There is a theorem stating that any 1D attractive potential, no matter how weak, always supports at least one bound state. For details, see Exercise 2.6.1.

In 3D, it is possible for an attractive potential to be too weak to support a bound state. Intuitively, this happens when the zero-point energy of a prospective ground state exceeds the well depth. The figure below shows a numerical example, calculated for a uniform 3D spherically symmetric well (the l's labeling the various curves are angular momentum quantum numbers). To learn more about this phenomenon, refer to Exercise 2.6.2.

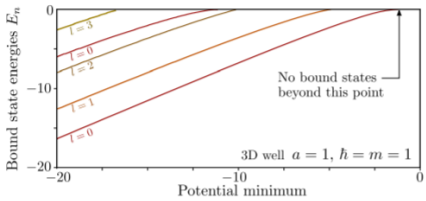

Figure 2.1.4

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2.2: Quasi-Bound States and Resonances

For the 1D finite square well, there is a clear distinction between bound and free states. Certain potentials, however, can host a special class of states called "**quasi-bound states**". Like a bound state, a quasi-bound state is localized in one region of space. However, it is an *approximate* eigenstate of the Hamiltonian that lies in the energy range of the free state continuum. As we shall see, quasi-bound states play an important important role in scattering experiments.

The figure below shows an example of a potential function that gives rise to quasi-bound states. In the exterior region, $|x| > b$, the potential is zero. Between $x = -b$ and $x = b$, there is a "barrier" of positive potential V_b. Embedded in the middle of this barrier, for $|x| < a$, is a central well of depth U, where $0 < V_b - U < V_b$.

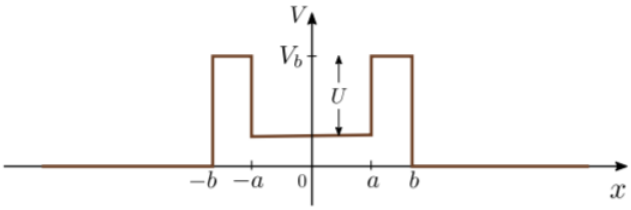

Figure 2.2.1

This potential is purely repulsive ($V \geq 0$ everywhere), so there are no true bound states. The only exact eigenstates of the Hamiltonian are free states.

However, there is something intriguing about the central well. Consider an alternative scenario where the potential in the exterior region is V_b rather than 0; i.e., the potential function is a finite square well:

$$V_{\text{alt}}(x) = \begin{cases} V_b - U, & |x| < a, \\ V_b, & \text{otherwise.} \end{cases} \tag{2.2.1}$$

In this case, there would be one or more bound states, in the energy range $V_b - U < E < V_b$. These bound states' wavefunctions diminish exponentially away from the well, and are thus close to zero for $|x| > b$. Since $V(x)$ and $V_{\text{alt}}(x)$ differ only in the region $|x| > b$, these wavefunctions ought to be *approximate* solutions to the Schrödinger wave equation for the original potential $V(x)$, which does not support bound states! Such approximate solutions are called quasi-bound states.

Let us analyze the potential $V(x)$ using the **scattering experiment** framework from the previous chapter. Consider an incident particle of energy $E > 0$ whose wavefunction is

$$\psi_i(x) = \Psi_i \, e^{ik_i x}. \tag{2.2.2}$$

This produces a scattered wavefunction $\psi_s(x)$ that is outgoing (as discussed in the previous chapter). In the exterior region, the scattered wavefunction takes the form

$$\psi_s(x) = \Psi_i \times \begin{cases} f_- \, e^{-ik_i x}, & x \leq -b \\ f_+ \, e^{ik_i x}, & x \geq b. \end{cases} \tag{2.2.3}$$

The scattering amplitudes f_+ and f_- can be found by solving the Schrödinger wave equation using the transfer matrix method (see Appendix B). The figure below shows numerical results obtained for $U = 20$, $V_b = 30$, $a = 1$, and $b = 1.2$ or $b = 1.4$, with $\hbar = m = 1$.

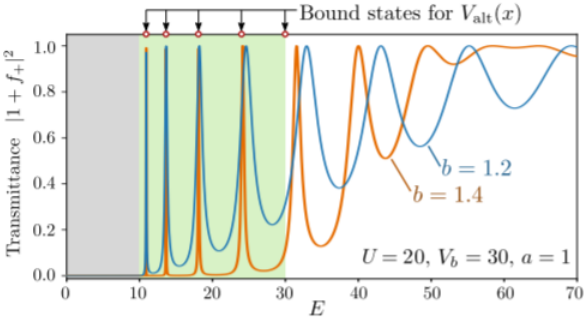

Figure 2.2.2

The vertical axis shows $|1+f_+|^2$, which is called the "transmittance" and corresponds to the probability for the incident particle to pass through the potential. The horizontal axis is the particle energy E. For $E < V_b - U$, the transmittance approaches zero, and for $E \gtrsim V_b$, the transmittance approaches unity, as expected. In the energy range $V_b - U < E \lesssim V_b$, the transmittance forms a series of narrow peaks. For larger b (i.e., when the central well is more isolated from the exterior space), the peaks are narrower. At the top of the figure, we have also plotted the bound state energies for the square well potential $V_{\text{alt}}(x)$. These energies closely match the locations of the transmittance peaks!

Upon examining the total wavefunction $\psi(x)$ at these special energies, we find other interesting features. The figure below plots $|\psi(x)|^2$ versus x at the energies of the first three transmittance peaks, along with the corresponding bound state wavefunctions for the square well V_{alt}. At each transmittance peak, $|\psi(x)|^2$ is much larger within the potential region, and its shape is very similar to a square well bound state.

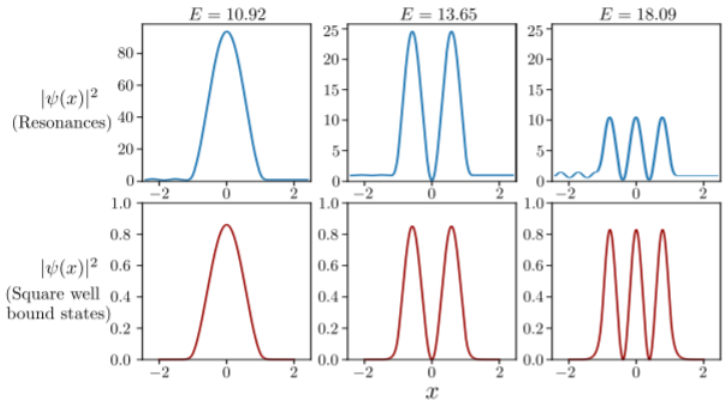

Figure 2.2.3

The enhancement of $|\psi(x)|^2$ is called a **resonance**. It happens because of the existence of a quasi-bound state—an approximate energy eigenstate localized in the scattering region. When an incident particle enters the scattering region with the right energy, it spends a long time trapped in the quasi-bound state, before eventually escaping back to infinity.

This is analogous to the phenomenon of resonance in a classical harmonic oscillator. When a damped harmonic oscillator is subjected to an oscillatory driving force, it settles into a steady-state oscillatory motion at the driving frequency. If the driving frequency matches the oscillator's natural frequency, the amplitude of the oscillation becomes large, and the system is said to be "resonant". In the quantum mechanical context, the incident wavefunction plays the role of a driving force, the incident particle energy is like the driving frequency, and the energy of a quasi-bound state is like a natural frequency of oscillation.

Resonances play a critical role throughout experimental physics. Experiments are often conducted for the express purpose of locating and studying resonances. When a resonance peak is found, its location and shape can be used to deduce various features of the quasi-bound state, which in turn supplies important information about the underlying system.

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2.3: Green's Function Analysis of Scattering Resonances

Quasi-bound states and resonances are not limited to 1D, but are equally (or more) important in 2D and 3D. A useful and general way to study them is the quantum Green's function formalism developed in the previous chapter.

Let $\hat{H} = \hat{T} + \hat{V}$ be the Hamiltonian of a system supporting resonances, where $\hat{T}$ is the kinetic energy operator and $\hat{V}$ is the potential operator. We decompose the potential into

$$\hat{V} = \hat{V}_0 + \hat{V}_1, \tag{2.3.1}$$

where $\hat{V}_0$ is a "confining potential" that supports a bound state, and $\hat{V}_1$ is a "deconfining potential" that turns the bound state into a quasi-bound state. The figure below shows an example of such a decomposition, for the 1D model from the previous section.

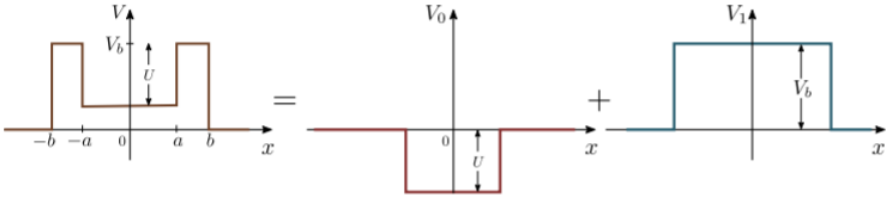

Figure 2.3.1

For the potential $\hat{V}_0$ (in the absence of $\hat{V}_1$), let there be a bound state $|\varphi\rangle$, with energy E_0. Furthermore, we assume that the potential supports a continuum of free states $\{|\psi_k\rangle\}$ with energies $\{E_k\}$, where k is some d-dimensional continuous index for the free states (analogous to the wave-vector for plane wave states). The bound state and free states satisfy the Schrödinger equation

$$\left(\hat{T} + \hat{V}_0\right)|\varphi\rangle = E_0|\varphi\rangle \tag{2.3.2}$$

$$\left(\hat{T} + \hat{V}_0\right)|\psi_k\rangle = E_k|\psi_k\rangle, \tag{2.3.3}$$

along with the orthogonality and completeness relations

$$\langle\varphi|\psi_k\rangle = 0, \quad |\varphi\rangle\langle\varphi| + \int d^d k\, |\psi_k\rangle\langle\psi_k| = \hat{I}. \tag{2.3.4}$$

As described in Section 1.7, the causal Green's function is

$$\hat{G}_0(E) = \lim_{\varepsilon \to 0^+} \left(E - \hat{T} - \hat{V}_0 + i\varepsilon\right)^{-1}. \tag{2.3.5}$$

Now introduce the deconfining potential $\hat{V}_1$. According to Dyson's equations (Section VI of the previous chapter), the Green's function for the full system is

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}_1\hat{G}_0. \tag{2.3.6}$$

We want the matrix elements of $\hat{G}(E)$, which can then be used to find scattering amplitudes. We will calculate them by using the states $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ as a basis—but note that this basis does *not* consist of energy eigenfunctions of the full Hamiltonian $\hat{H}$. In particular, $|\varphi\rangle$ is not an exact eigenstate of $\hat{H}$.

As usual when dealing with Dyson's equations, we must watch out for the fact that $\hat{G}$ appears on both the left and right hand sides. This can be dealt with by judiciously inserting a resolution of the identity:

$$\begin{aligned} \hat{G} &= \hat{G}_0 + \hat{G}\hat{I}\hat{V}_1\hat{G}_0 \\ &= \hat{G}_0 + \hat{G}\left(|\varphi\rangle\langle\varphi| + \int d^d k\, |\psi_k\rangle\langle\psi_k|\right)\hat{V}_1\hat{G}_0. \end{aligned} \tag{2.3.7}$$

We now compute the matrix element $\langle\varphi|\cdots|\varphi\rangle$ for both sides of the equation:

$$
\begin{aligned}
\langle\varphi|\hat{G}|\varphi\rangle &= \langle\varphi|\hat{G}_0|\varphi\rangle \ + \langle\varphi|\hat{G}|\varphi\rangle \langle\varphi|\hat{V}_1\hat{G}_0|\varphi\rangle + \int d^dk \, \langle\varphi|\hat{G}|\psi_k\rangle \langle\psi_k|\hat{V}_1\hat{G}_0|\varphi\rangle \\
\langle\varphi|\hat{G}|\varphi\rangle \left(1 - \langle\varphi|\hat{V}_1\hat{G}_0|\varphi\rangle\right) &= \langle\varphi|\hat{G}_0|\varphi\rangle + \int d^dk \, \langle\varphi|\hat{G}|\psi_k\rangle \langle\psi_k|\hat{V}_1\hat{G}_0|\varphi\rangle \\
\lim_{\varepsilon\to 0^+} \langle\varphi|\hat{G}|\varphi\rangle \left(1 - \frac{\langle\varphi|\hat{V}_1|\varphi\rangle}{E - E_0 + i\varepsilon}\right) &= \lim_{\varepsilon\to 0^+} \frac{1}{E - E_0 + i\varepsilon} \left(1 + \int d^dk \, \langle\varphi|\hat{G}|\psi_k\rangle \langle\psi_k|\hat{V}_1|\varphi\rangle\right) \\
\lim_{\varepsilon\to 0^+} \langle\varphi|\hat{G}|\varphi\rangle \Big(E - E_0 - \langle\varphi|\hat{V}_1|\varphi\rangle \ + i\varepsilon\Big) &- \int d^dk \, \langle\varphi|\hat{G}|\psi_k\rangle \langle\psi_k|\hat{V}_1|\varphi\rangle = 1. \qquad (2.3.8)
\end{aligned}
$$

Similarly, computing the matrix element $\langle\varphi|\cdots|\psi_k\rangle$ gives:

$$
\begin{aligned}
\langle\varphi|\hat{G}|\psi_k\rangle \ &= \langle\varphi|\hat{G}_0|\psi_k\rangle + \langle\varphi|\hat{G}|\varphi\rangle \langle\varphi|\hat{V}_1\hat{G}_0|\psi_k\rangle + \int d^dk' \, \langle\varphi|\hat{G}|\psi_{k'}\rangle \langle\psi_{k'}|\hat{V}_1\hat{G}_0|\psi_k\rangle \\
&= \lim_{\varepsilon\to 0^+} \left(E - E_k + i\varepsilon\right)^{-1} \left(\langle\varphi|\hat{G}|\varphi\rangle \langle\varphi|\hat{V}_1|\psi_k\rangle + \int d^dk' \, \langle\varphi|\hat{G}|\psi_{k'}\rangle \langle\psi_{k'}|\hat{V}_1|\psi_k\rangle\right). \qquad (2.3.9)
\end{aligned}
$$

The equations thus far have been exact (we have *not* used perturbation theory). Now we apply an approximation: in the last line of the above equation, let the factor of $\langle\varphi|G|\varphi\rangle$ be large, so that the first term in the sum becomes dominant. It will be shown below that $\langle\varphi|G|\varphi\rangle$ being large is precisely the resonance condition, so this approximation will be self-consistent. With this, we obtain

$$
\langle\varphi|\hat{G}|\psi_k\rangle \approx \lim_{\varepsilon\to 0^+} \frac{\langle\varphi|\hat{G}|\varphi\rangle \langle\varphi|\hat{V}_1|\psi_k\rangle}{E - E_k + i\varepsilon}. \qquad (2.3.10)
$$

Combining this with Equation (2.3.8) gives

$$
\lim_{\varepsilon\to 0^+} \left[\langle\varphi|\hat{G}|\varphi\rangle \left(E - E_0 - \langle\varphi|\hat{V}_1|\varphi\rangle \ + i\varepsilon\right) - \int d^dk \, \frac{\langle\varphi|\hat{G}|\varphi\rangle\langle\varphi|\hat{V}_1|\psi_k\rangle}{E - E_k + i\varepsilon} \langle\psi_k|\hat{V}_1|\varphi\rangle\right] \approx 1. \qquad (2.3.11)
$$

Hence,

Definition: Resonance Condition

$$
\begin{aligned}
\langle\varphi|\,\hat{G}(E)\,|\varphi\rangle &\approx \frac{1}{E - E_0 - \langle\varphi|V_1|\varphi\rangle - \Sigma(E)} \\
\text{where} \quad \Sigma(E) &\equiv \lim_{\varepsilon\to 0^+} \int d^dk \, \frac{|\langle\psi_k|\hat{V}_1|\varphi\rangle|^2}{E - E_k + i\varepsilon}.
\end{aligned} \qquad (2.3.12)
$$

The quantity $\Sigma(E)$ is called the **self-energy**, and we will have more to say about it shortly. It depends on E, but let us assume for now that the dependence is weak, so that Σ can be effectively treated as a constant. It is complex-valued, and both its real and imaginary parts are important; we will shortly show that $\mathrm{Im}(\Sigma) < 0$.

From Equation (2.3.12), we can see that $\langle\varphi|\hat{G}(E)|\varphi\rangle$ is large when the denominator is as close to zero as possible. This is called the **resonance condition**, and is self-consistent with the approximation that we made in the above derivation. As we vary the incident energy E over the range of real values, the resonance condition is satisfied when

$$
E \ \approx \ E_{\text{res}} \ \equiv \ E_0 + \langle\varphi|\hat{V}_1|\varphi\rangle + \mathrm{Re}\big[\,\Sigma\,\big]. \qquad (2.3.13)
$$

We call E_{res} the **resonance energy**. Its first term is the energy of the original bound state, in the absence of the deconfining potential $\hat{V}_1$. The second term is the energy shift induced by $\hat{V}_1$. The third term is equal to the real part of the self-energy Σ, and has a more subtle meaning. Since the definition of Σ involves $\{|\psi_k\rangle\}$, we can think of this term as an energy shift induced by the continuum of free states.

In Section 1.8, we derived the following relationship between the Green's function and the scattering amplitude f:

$$
f(\mathbf{k} \to \mathbf{k}') \ \propto \ \langle\mathbf{k}'|\hat{V}|\mathbf{k}\rangle + \langle\mathbf{k}'|\hat{V}\hat{G}\hat{V}|\mathbf{k}\rangle. \qquad (2.3.14)
$$

Here, $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ are incident and scattered plane-wave states satisfying $|\mathbf{k}| = |\mathbf{k}'|$. The first term describes the lowest-order scattering process (the first Born approximation). The second term contains all second- and higher-order scattering processes. By

inserting resolutions of the identity between each $\hat{V}$ and $\hat{G}$ operator in the second term, we find that f contains a contribution of the form

$$\Delta f(\mathbf{k} \to \mathbf{k}') \;\propto\; \langle \mathbf{k}'|\hat{V}|\varphi\rangle\langle\varphi|\hat{G}|\varphi\rangle\langle\varphi|\hat{V}|\mathbf{k}\rangle \;=\; \frac{\langle \mathbf{k}'|\hat{V}|\varphi\rangle\,\langle\varphi|\hat{V}|\mathbf{k}\rangle}{E - E_{\text{res}} - i\text{Im}[\,\Sigma\,]}. \tag{2.3.15}$$

At resonance, the denominator becomes small and hence Δf should be the dominant contribution to f. It is worth emphasizing that Δf is extracted from a combination of *all* terms in the Born series, not just low-order terms. Intuitively, we can think of a resonant scattering scenario as one where the particle bounces around inside the potential many times before it finally escapes—i.e., high orders in the Born series are significant.

The figure below shows the energy dependence of Δf, according to Equation (2.3.15):

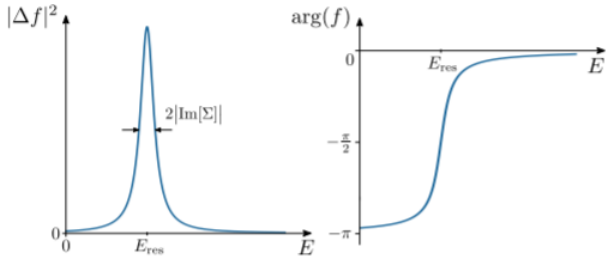

Figure 2.3.2

The graph of $|\Delta f|^2$ versus E has a shape known as a **Lorentzian**. It has a peak centered at the resonance energy E_{res}. The peak width is characterized by the **full-width at half-maximum** (FWHM), the spacing between the two energies where $|\Delta f|^2$ is at half its maximum value:

$$\delta E^{(\text{FWHM})} = 2\,\Big|\text{Im}[\Sigma]\Big|. \tag{2.3.16}$$

Thus, the closer the self-energy gets to being a real quantity, the sharper the peak.

The phase $\arg[\Delta f]$ also contains useful information. As E crosses E_{res} from below, the phase increases by π. The energy range over which this phase shift occurs is $\sim |\text{Im}[\Sigma]|$.

These two signatures—peaks and phase shifts—are sought after in numerous real-world scattering experiments. In actual experiments, the peaks and phase shifts are often overlaid on a "background" caused by non-resonant effects. For example, the plot below was released by the CMS experiment at the Large Hadron Collider (LHC), showing a resonance peak on a large background. This was part of the evidence for the LHC's discovery of a new particle, the Higgs boson, in 2012.

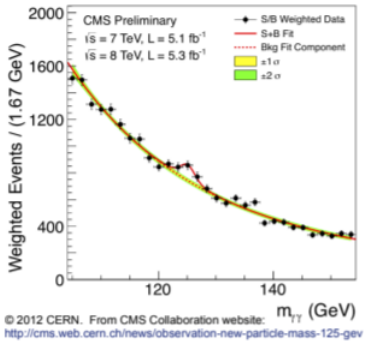

Figure 2.3.3

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2.4: Fermi's Golden Rule

We have seen that the width of a resonance is determined by the imaginary part of the self-energy, $\mathrm{Im}[\Sigma]$. In this section, we will show that $\mathrm{Im}[\Sigma]$ has a physical meaning: it represents the **decay rate** of a quasi-bound state. Moreover, it can be approximated using a simple but important formula known as **Fermi's Golden Rule**.

Suppose we set the quantum state of a particle to a quasi-bound state $|\varphi\rangle$ at some initial time $t=0$. Since $|\varphi\rangle$ is not an exact eigenstate of the Hamiltonian, the particle will not remain in that state under time evolution. For $t>0$, its wavefunction should become less and less localized, which can be interpreted as the escape of the particle to infinity or the "decay" of the quasi-bound state into the free state continuum.

The decay process can be described by

$$P(t)=\left|\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\right|^2, \tag{2.4.1}$$

which is the probability for the system to continue occupying state $|\varphi\rangle$ after time t. In order to calculate $P(t)$, let us define the function

$$f(t)=\begin{cases}\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\, e^{-\varepsilon t}, & t\geq 0\\ 0, & t<0,\end{cases} \tag{2.4.2}$$

where $\varepsilon\in\mathbb{R}^+$. For $t\geq 0$ and $\varepsilon\to 0^+$, we see that $|f(t)|^2\to P(t)$. The reason we deal with $f(t)$ is that it is more well-behaved than the actual amplitude $\langle\varphi|\exp(-i\hat{H}t/\hbar)|\varphi\rangle$. The function is designed so that firstly, it vanishes at negative times prior to start of our thought experiment; and secondly, it vanishes as $t\to\infty$ due to the "regulator" ε. The latter enforces the idea that the bound state decays permanently into the continuum of free states, and is never re-populated by waves "bouncing back" from infinity.

We can determine $f(t)$ by first studying its Fourier transform,

$$F(\omega)\;=\;\int_{-\infty}^{\infty}dt\;e^{i\omega t}\,f(t)\;=\;\int_0^{\infty}dt\;e^{i(\omega+i\varepsilon)t}\;\langle\varphi|e^{-i\hat{H}t/\hbar}|\varphi\rangle. \tag{2.4.3}$$

Now insert a resolution of the identity, $\hat{I}=\sum_n|n\rangle\langle n|$, where $\{|n\rangle\}$ denotes the exact eigenstates of $\hat{H}$ (for free states, the sum goes to an integral in the usual way):

$$\begin{aligned}F(\omega)&=\int_0^{\infty}dt\;e^{i(\omega+i\varepsilon)t}\;\sum_n\langle\varphi|e^{-i\hat{H}t/\hbar}|n\rangle\langle n|\varphi\rangle\\&=\sum_n\langle\varphi|n\rangle\left(\int_0^{\infty}dt\;\exp\left[i\left(\omega-\frac{E_n}{\hbar}+i\varepsilon\right)t\right]\right)\langle n|\varphi\rangle\\&=\sum_n\langle\varphi|n\rangle\frac{i}{\omega-\frac{E_n}{\hbar}+i\varepsilon}\langle n|\varphi\rangle\\&=i\hbar\,\langle\varphi|\left(\hbar\omega-\hat{H}+i\hbar\varepsilon\right)^{-1}|\varphi\rangle.\end{aligned} \tag{2.4.4}$$

In the third line, the regulator ε removes any contribution from the $t\to\infty$ limit of the integral, in accordance with our requirement that the decay of the bound state is permanent. Hence, we obtain

$$\lim_{\varepsilon\to 0^+}F(\omega)=i\hbar\,\langle\varphi|\hat{G}(\hbar\omega)|\varphi\rangle, \tag{2.4.5}$$

where $\hat{G}$ is our old friend the causal Green's function. The fact that the *causal* Green's function shows up is due to our definition of $f(t)$, which vanishes for $t<0$.

As discussed in the previous section, when the resonance condition is satisfied,

$$\langle\varphi|\,\hat{G}(E)\,|\varphi\rangle\approx\frac{1}{E-E_{\mathrm{res}}-i\mathrm{Im}[\Sigma]}, \tag{2.4.6}$$

where E_{res} is the resonance energy and Σ is the self-energy of the quasi-bound state. We can now perform the inverse Fourier transform

$$\begin{aligned}\lim_{\varepsilon\to 0^+} f(t) &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,e^{-i\omega t}\,F(\omega)\\ &= \frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\,\frac{e^{-i\omega t}}{\omega-(E_{\rm res}+i{\rm Im}[\Sigma])/\hbar}\\ &= \exp\!\left(-\frac{iE_{\rm res}t}{\hbar}\right)\,\exp\!\left(-\frac{|{\rm Im}[\Sigma]|}{\hbar}\,t\right).\end{aligned} \tag{2.4.7}$$

In deriving the last line, we performed a contour integration assuming that ${\rm Im}[\Sigma]<0$; this assumption will be proven shortly. The final result is

$$P(t)=e^{-\kappa t},\quad \text{where}\ \ \kappa=\frac{2|{\rm Im}[\Sigma]|}{\hbar}. \tag{2.4.8}$$

Let us now take a closer look at the self-energy. From our earlier definition,

$$\Sigma(E)\equiv\lim_{\varepsilon\to 0^+}\int d^dk\,\frac{|\langle\psi_k|\hat{V}_1|\varphi\rangle|^2}{E-E_k+i\varepsilon}, \tag{2.4.9}$$

where $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ are the bound and free states of the model in the absence of $\hat{V}_1$, and E_k is the energy of the k-th free state. The imaginary part is

$$\begin{aligned}{\rm Im}\big[\Sigma(E)\big] &= \lim_{\varepsilon\to 0^+}\int d^dk\,\Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\,{\rm Im}\left(\frac{1}{E-E_k+i\varepsilon}\right)\\ &= -\int d^dk\,\Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\,\left[\lim_{\varepsilon\to 0^+}\,\frac{\varepsilon}{(E-E_k)^2+\varepsilon^2}\right].\end{aligned} \tag{2.4.10}$$

The quantity inside the square brackets is a Lorentzian function, which is always positive; hence, ${\rm Im}(\Sigma)<0$, as previously asserted. The Lorentzian function has the limiting form

$$\lim_{\varepsilon\to 0^+}\,\frac{\varepsilon}{x^2+\varepsilon^2}=\pi\delta(x). \tag{2.4.11}$$

This comes from the fact that as $\varepsilon\to 0^+$, the Lorentzian curve describes a sharper and sharper peak, but the area under the curve is fixed as π. Hence,

$${\rm Im}\big[\Sigma(E)\big]=-\pi\int d^dk\,\Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\,\delta(E-E_k). \tag{2.4.12}$$

Because of the delta function, we see that the only non-vanishing contributions to the integral come from the parts of k-space where $E=E_k$.

We can further simplify the result by defining the **density of states**,

$$\mathcal{D}(E)=\int d^dk\,\delta(E-E_k). \tag{2.4.13}$$

Roughly speaking, this measures the number of free states that exist at energy E. The k-space volume d^dk is proportional to the number of free states at each k, while the delta function restricts the contributions to only those free states with energy E. (In the next section, we'll see an explicit example of how to calculate $\mathcal{D}(E)$.) Now, for any function $f(k)$,

$$\int d^dk\,f(k)\,\delta(E-E_k)=\overline{f(k(E))}\,\mathcal{D}(E), \tag{2.4.14}$$

where $\overline{f(k(E))}$ denotes the mean value of $f(k)$ for the free states satisfying $E_k=E$. Applying this to the imaginary part of the self-energy gives

$${\rm Im}\big[\Sigma(E)\big]=-\pi\,\overline{\Big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\Big|^2}\,\mathcal{D}(E). \tag{2.4.15}$$

Hence, the quasi-bound state's decay rate is

Definition: Fermi's Golden Rule

$$\kappa = -\frac{2}{\hbar}\mathrm{Im}\big[\Sigma(E_{\rm res})\big] = \frac{2\pi}{\hbar}\,\overline{\left|\langle\psi_{k(E_{\rm res})}|\hat{V}_1|\varphi\rangle\right|^2}\,\mathcal{D}(E_{\rm res}). \tag{2.4.16}$$

This extremely important result is called **Fermi's golden rule**. It says that the decay rate of a quasi-bound mode is directly proportional to two factors. The first factor describes how strongly $\hat{V}_1$ couples the quasi-bound state and the free states, as determined by the quantity $\langle\psi_k|\hat{V}_1|\varphi\rangle$, called the **transition amplitude**. It goes to zero when $\hat{V}_1 = 0$, which is the case where $|\varphi\rangle$ is a true bound state that does not decay. The second factor is the density of free states, and describes how many free states are available for $|\varphi\rangle$ to decay into. Both factors depend on energy, and must be evaluated at the resonance energy $E_{\rm res}$.

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2.5: Fermi's Golden Rule in a 1D Resonance Model

Fermi's golden rule can be used to study a wide variety of quantum systems, and we will see examples of its usefulness in subsequent chapters. In this section, we will apply it to the simple 1D model from Section 2.2, and evaluate how well it works. The model potential is

$$\begin{aligned} &V(x) = V_0(x) + V_1(x), \quad \text{where} \\ &V_0(x) = -U\,\Theta(a-|x|), \quad V_1(x) = V_b\,\Theta(b-|x|), \quad 0 < U < V_b. \end{aligned} \tag{2.5.1}$$

The potential well V_0 supports one or more bound states. For simplicity, we focus on the ground state, whose energy E_0 lies in the range $[-U, 0]$. Once V_1 is introduced, this will turn into the lowest quasi-bound state, with resonance energy $E_{\rm res} \approx E_0 + V_b > 0$.

When the potential consists only of V_0, the ground state wavefunction can be obtained by solving the Schrödinger wave equation for the boundary condition $\varphi(x) \to 0$ as $|x| \to \infty$. It has the form

$$\varphi(x) = \begin{cases} \mathcal{A}\,\cos(qx), & |x| < a \\ \mathcal{B}\,\exp(-\eta|x|), & |x| \geq a, \end{cases} \tag{2.5.2}$$

where $\mathcal{A}$ and $\mathcal{B}$ are constants to be determined, and

$$q = \sqrt{\frac{2m}{\hbar^2}(E_0+U)}, \quad \eta = \sqrt{\frac{2m}{\hbar^2}|E_0|}. \tag{2.5.3}$$

By matching both $\varphi(x)$ and $d\varphi/dx$ across the $x = a$ interface, we can derive a transcendental equation for E_0, which can be solved numerically. Once we know E_0, we also know q and η. We can then relate $\mathcal{A}$ and $\mathcal{B}$ by matching $\varphi(x)$ across the $x = a$ interface:

$$\mathcal{A} = \mathcal{B}\,\frac{\exp(-\eta a)}{\cos(qa)}. \tag{2.5.4}$$

Moreover, the wavefunction must be normalized to unity:

$$\begin{aligned} 1 \;&= \mathcal{A}^2 \int_{-a}^{a} \cos^2(qx) + 2\mathcal{B}^2 \int_a^\infty dx\;\exp(-2\eta x) \\ &= \mathcal{A}^2 \left(a + \frac{\sin(2qa)}{2q} \right) + \mathcal{B}^2\,\frac{\exp(-2\eta a)}{\eta}. \end{aligned} \tag{2.5.5}$$

Putting the last two equations together yields

$$\mathcal{B}^2 = \frac{\exp\left(2\eta a\right)}{a} \left[\frac{1+\sin(2qa)/2qa}{\cos^2(qa)} + \frac{1}{\eta a} \right]^{-1}. \tag{2.5.6}$$

We now wish to compute the transition amplitude

$$\langle \psi_k | \hat{V}_1 | \varphi \rangle \;=\; \int_{-\infty}^{\infty} dx\;\psi_k^*(x)\,V_1(x)\,\varphi(x) \;=\; V_b \int_{-b}^{b} dx\;\psi_k^*(x)\,\varphi(x), \tag{2.5.7}$$

where $\psi_k(x)$ is the wavefunction of a free state for the system with potential $V_0(x)$, which is labeled by some continuous index k. We can use a trick to avoid calculating the exact form of $\psi_k(x)$. Because $\psi_k(x)$ and $\varphi(x)$ must be orthogonal,

$$\int_{-b}^{b} dx\;\psi_k^*(x)\,\varphi(x) = -\int_{|x|>a} dx\;\psi_k^*(x)\,\varphi(x). \tag{2.5.8}$$

When evaluating the free states outside the potential well, we can approximate them as the free states of the particle without the potential well, i.e., simple plane waves:

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}}\,e^{ikx}, \quad k \in \mathbb{R}, \quad |x| > a. \tag{2.5.9}$$

We likewise approximate their energies by $E_k \approx \hbar^2 k^2/2m$. Plugging $\psi_k(x)$ into the formula for the transition amplitude, and performing the necessary integrals, yields

$$\langle \psi_k | \hat{V}_1 | \varphi \rangle \;=\; -\mathcal{B}\sqrt{\frac{2}{\pi}}\,\frac{\hbar^2}{2m}\,\big[\eta\cos(kb) - k\sin(kb)\big]\;\exp(-\eta b). \tag{2.5.10}$$

Within Fermi's golden rule, we must use a value of k such that

$$E_k = E_{\rm res} \approx E_0 + V_b \quad\Rightarrow\quad k \approx \sqrt{\frac{2m}{\hbar^2}(E_0 + V_b)}\,. \tag{2.5.11}$$

The next thing that we need to calculate is the density of free states. This can be done by once again taking $E_k \approx \hbar^2 k^2/2m$, and performing a change of variables:

$$\begin{aligned}\mathcal{D}(E) \;&=\; \int_{-\infty}^{\infty} dk\;\delta\left(E - \frac{\hbar^2 k^2}{2m}\right) \\ &= 2\cdot\int_0^{\infty} dE'\;\frac{dk}{dE'}\;\delta(E - E') \\ &= \sqrt{\frac{2m}{\hbar^2 E}}.\end{aligned} \tag{2.5.12}$$

Note the factor of 2 on the second line; it is there because there is both a positive and a negative value of k for each E.

Having obtained expressions for the transition amplitude and the density of states, we just have to plug them into Fermi's golden rule to obtain the decay rate κ. The figure below shows how κ varies with the barrier thickness $b-a$, with all other model parameters fixed ($U = 20, V_b = 30, a = 1$):

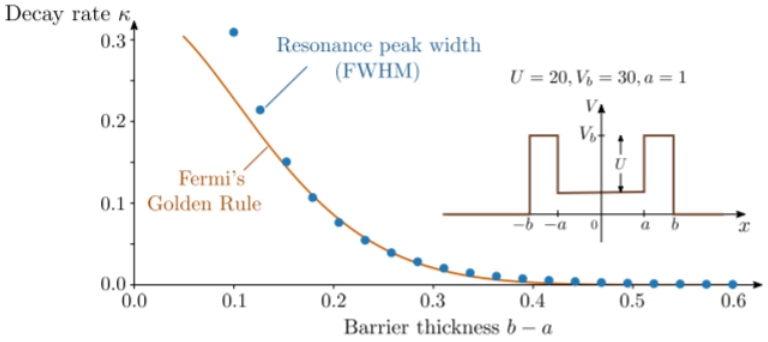

Figure 2.5.1

For comparison, the figure also plots the width of the resonant scattering peak, which according to our preceding discussion is supposed to be equal to κ. To obtain these values, we use the transfer matrix method to compute the E-dependent transmittance for particles incident on one side of the potential (see Appendix B). The transmittance is peaked near $E_{\rm res}$, and the full-width at half-maximum (see Section 2.3) is estimated numerically. The results are shown as blue dots in the figure.

We see that Fermi's golden rule generally agrees well with the results from the transfer matrix method. There is some discrepancy, notably when the barrier is thin. Remember that Fermi's golden rule relies on the approximation that the quasi-bound state is strongly confined (i.e., having $\langle\varphi|G|\varphi\rangle$ be large in the derivations of Sections 2.3 and 2.4). Moreover, we have approximated the free states $|\psi_k\rangle$ using the plane wave states in the absence of any potential, which is an assumption commonly employed when using Fermi's golden rule.

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2.6: Exercises

Exercises

Exercise 2.6.1

Use the variational theorem to prove that a 1D potential well has at least one bound state. Assume that the potential $V(x)$ satisfies (i) $V(x) < 0$ for all x, and (ii) $V(x) \to 0$ for $x \to \pm\infty$. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{2.6.1}$$

Consider a (real) trial wavefunction

$$\psi(x;\gamma) = \left(\frac{2\gamma}{\pi}\right)^{1/4} e^{-\gamma x^2}. \tag{2.6.2}$$

Note that this can be shown to be normalized to unity, using Gauss' integral

$$\int_{-\infty}^{\infty} dx\; e^{-2\gamma x^2} = \sqrt{\frac{\pi}{2\gamma}}. \tag{2.6.3}$$

Now prove that

$$\begin{aligned} \langle E\rangle &= \int_{-\infty}^{\infty} dx\; \psi(x)\,\hat{H}\,\psi(x) \\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx \left(\frac{d\psi}{dx}\right)^2 + \int_{-\infty}^{\infty} dx\; V(x)\,\psi^2(x) \\ &= A\sqrt{\gamma}\left[\sqrt{\gamma} + B\int_{-\infty}^{\infty} dx\; V(x)\; e^{-\gamma x^2}\right], \end{aligned} \tag{2.6.4}$$

where A and B are positive real constants to be determined. By looking at the quantity in square brackets in the limit $\gamma \to 0$, argue that $\langle E\rangle < 0$ in this limit. Hence, explain why this implies the existence of a bound state.

Finally, try generalizing this approach to the case of a 2D radially-symmetric potential well $V(x,y) = V(r)$, where $r = \sqrt{x^2+y^2}$. Identify which part of the argument fails in 2D. [For a discussion of certain 2D potential wells that *do* always support bounds states, similar to 1D potential wells, see Simon (1976).]

Exercise 2.6.2

In this problem, you will investigate the existence of bound states in a 3D potential well that is finite, uniform, and spherically-symmetric. The potential function is

$$V(r,\theta,\phi) = -U\Theta(a-r), \tag{2.6.5}$$

where a is the radius of the spherical well, U is the depth, and (r,θ,ϕ) are spherical coordinates defined in the usual way.

The solution involves a variant of the partial wave analysis discussed in Appendix A. For $E < 0$, the Schrödinger equation reduces to

$$\begin{cases} \left(\nabla^2 + q^2\right)\psi(r,\theta,\phi) = 0 \;\text{ where }\; q = \sqrt{2m(E+U)/\hbar^2}, & \text{for } r \le a \\ \left(\nabla^2 - \gamma^2\right)\psi(r,\theta,\phi) = 0 \;\text{ where }\; \gamma = \sqrt{-2mE/\hbar^2}, & \text{for } r \ge a. \end{cases} \tag{2.6.6}$$

For the first equation (called the Helmholtz equation), we seek solutions of the form

$$\psi(r,\theta,\phi) = f(r)\,Y_{\ell m}(\theta,\phi), \tag{2.6.7}$$

where $Y_{\ell m}(\theta,\phi)$ are spherical harmonics, and the integers l and m are angular momentum quantum numbers satisfying $l \ge 0$ and $-l \le m \le l$. Substituting into the Helmholtz equation yields

$$r^2 \frac{d^2 f}{dr^2} + 2r \frac{df}{dr} + \left[q^2 r^2 - l(l+1) \right] f(r) = 0, \tag{2.6.8}$$

which is the **spherical Bessel equation**. The solutions to this equation that are non-divergent at $r = 0$ are $f(r) = j_\ell(qr)$, where j_ℓ is called a **spherical Bessel function of the first kind**. Most numerical packages provide functions to calculate these (e.g., `scipy.special.spherical_jn` in Scientific Python).

Similarly, solutions for the second equation can be written as $\psi(r, \theta, \phi) = g(r)\, Y_{\ell m}(\theta, \phi)$, yielding an equation for $g(r)$ called the **modified spherical Bessel equation**. The solutions which do not diverge as $r \to \infty$ are $g(r) = k_\ell(\gamma r)$, where k_ℓ is called a **modified spherical Bessel function of the second kind**. Again, this can be computed numerically (e.g., using `scipy.special.spherical_kn` in Scientific Python).

Using the above facts, show that the condition for a bound state to exist is

$$\frac{q j'_\ell(qa)}{j_\ell(qa)} = \frac{\gamma k'_\ell(\gamma a)}{k_\ell(\gamma a)}, \tag{2.6.9}$$

where j'_ℓ and k'_ℓ denote the derivatives of the relevant special functions, and q and γ depend on E and U as described above. Write a program to search for the bound state energies at any given a and U, and hence determine the conditions under which the potential does not support bound states.

Further Reading

[1] Bransden & Joachain, §4.4, 9.2–9.3, 13.4

[2] Sakurai, §5.6, 7.7–7.8

[3] R. Courant and D. Hilbert, *Methods of Mathematical Physics* vol. 1, Interscience (1953).

[4] B. Simon, *The bound state of weakly coupled Schrödinger operators in one and two dimensions*, Annals of Physics **97**, 279 (1976).

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CHAPTER OVERVIEW

3: Quantum Entanglement

They don’t think it be like it is,
but it do.

Oscar Gamble

3.1: Quantum States of Multi-Particle Systems
3.2: Partial Measurements
3.3: The Einstein-Podolsky-Rosen "Paradox"
3.4: Bell's Theorem
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3.1: Quantum States of Multi-Particle Systems

So far, we have studied quantum mechanical systems consisting of single particles. The next important step is to look at systems of more than one particle. We shall see that the postulates of quantum mechanics, when applied to multi-particle systems, give rise to interesting and counterintuitive phenomena such as **quantum entanglement**.

Suppose we have two particles labeled A and B. If each individual particle is treated as a quantum system, the postulates of quantum mechanics require that its state be described by a vector in a Hilbert space. Let $\mathscr{H}_A$ and $\mathscr{H}_B$ denote the respective single-particle Hilbert spaces. Then the Hilbert space for the combined system of two particles is

$$\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B. \tag{3.1.1}$$

The symbol $\otimes$ refers to a **tensor product**, a mathematical operation that combines two Hilbert spaces to form another Hilbert space. It is most easily understood in terms of explicit basis vectors: let $\mathscr{H}_A$ be spanned by a basis $\{|\mu_1\rangle, |\mu_2\rangle, |\mu_3\rangle, \ldots\}$, and $\mathscr{H}_B$ be spanned by $\{|\nu_1\rangle, |\nu_2\rangle, |\nu_3\rangle, \ldots\}$. Then $\mathscr{H}_A \otimes \mathscr{H}_B$ is a space spanned by basis vectors consisting of *pairwise combinations* of basis vectors drawn from the $\mathscr{H}_A$ and $\mathscr{H}_B$ bases:

$$\Big\{ \ |\mu_i\rangle \otimes |\nu_j\rangle \ \text{ for all } \ |\mu_i\rangle, \ |\nu_j\rangle \ \Big\}. \tag{3.1.2}$$

Thus, if $\mathscr{H}_A$ has dimension d_A and $\mathscr{H}_B$ has dimension d_B, then $\mathscr{H}_A \otimes \mathscr{H}_B$ has dimension $d_A d_B$. Any two-particle state can be written as a superposition of these basis vectors:

$$|\psi\rangle = \sum_{ij} c_{ij} \, |\mu_i\rangle \otimes |\nu_j\rangle. \tag{3.1.3}$$

The inner product between the tensor product basis states is defined as follows:

$$\Big(|\mu_i\rangle \otimes |\nu_j\rangle \ , \ |\mu_p\rangle \otimes |\nu_q\rangle\Big) \ \equiv \ \Big(\langle\mu_i| \otimes \langle\nu_j|\Big)\Big(|\mu_p\rangle \otimes |\nu_q\rangle\Big) \ \equiv \ \langle\mu_i|\mu_p\rangle \, \langle\nu_j|\nu_q\rangle = \delta_{ip}\delta_{jq}. \tag{3.1.4}$$

In other words, the inner product is performed "slot-by-slot". We calculate the inner product for A, calculate the inner product for B, and then multiply the two resulting numbers. You can check that this satisfies all the formal requirements for an inner product in linear algebra (see Exercise 3.9.1).

For example, suppose $\mathscr{H}_A$ and $\mathscr{H}_B$ are both 2D Hilbert spaces describing spin-$1/2$ degrees of freedom. Each space can be spanned by an orthonormal basis $\{\,|{+z}\rangle, |{-z}\rangle\,\}$, representing "spin-up" and "spin-down". Then the tensor product space $\mathscr{H}$ is a 4D space spanned by

$$\Big\{ \ |{+z}\rangle \otimes |{+z}\rangle \, , \ |{+z}\rangle \otimes |{-z}\rangle \, , \ |{-z}\rangle \otimes |{+z}\rangle \, , \ |{-z}\rangle \otimes |{-z}\rangle \ \Big\}. \tag{3.1.5}$$

We now make an important observation. If A is in state $|\mu\rangle$ and B is in state $|\nu\rangle$, then the state of the combined system is fully specified: $|\mu\rangle \otimes |\nu\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$. But the reverse is not generally true! There exist states of the combined system that *cannot* be expressed in terms of definite states of the individual particles. For example, consider the following quantum state of two spin-$1/2$ particles:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|{+z}\rangle \otimes |{-z}\rangle \ - \ |{-z}\rangle \otimes |{+z}\rangle\Big). \tag{3.1.6}$$

This state is constructed from two of the four basis states in (3.1.5), and you can check that the factor of $1/\sqrt{2}$ ensures the normalization $\langle\psi|\psi\rangle = 1$ with the inner product rule (3.1.4). It is evident from looking at Equation (3.1.6) that neither A nor B possesses a definite $|{+z}\rangle$ or $|{-z}\rangle$ state. Moreover, we shall show (in Section 3.7) that there's *no* choice of basis that allows this state to be expressed in terms of definite individual-particle states; i.e.,

$$|\psi\rangle \neq |\psi_A\rangle \otimes |\psi_B\rangle \quad \text{for any} \ \ |\psi_A\rangle \in \mathscr{H}_A, \ |\psi_B\rangle \in \mathscr{H}_B. \tag{3.1.7}$$

In such a situation, the two particles are said to be **entangled**.

It is cumbersome to keep writing $\otimes$ symbols, so we will henceforth omit the $\otimes$ in cases where the tensor product is obvious. For instance,

$$\frac{1}{\sqrt{2}}\Big(|{+z}\rangle \otimes |{-z}\rangle \ - \ |{-z}\rangle \otimes |{+z}\rangle\Big) \ \equiv \ \frac{1}{\sqrt{2}}\Big(|{+z}\rangle|{-z}\rangle \ - \ |{-z}\rangle|{+z}\rangle\Big). \tag{3.1.8}$$

For systems of more than two particles, quantum states can be defined using multiple tensor products. Suppose a quantum system contains N particles described by the individual Hilbert spaces $\{\mathscr{H}_1, \mathscr{H}_2, \ldots, \mathscr{H}_N\}$ having dimensionality $\{d_1, \ldots, d_N\}$. Then the overall system is described by the Hilbert space

$$\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N, \tag{3.1.9}$$

which has dimensionality $d = d_1 d_2 \cdots d_N$. The dimensionality scales exponentially with the number of particles! For instance, if each particle has a 2D Hilbert space, a 20-particle system has a Hilbert space with $2^{20} = 1\,048\,576$ dimensions. Thus, even in quantum systems with a modest number of particles, the quantum state can carry huge amounts of information. This is one of the motivations behind the active research field of quantum computing.

Finally, a proviso: although we refer to subsystems like A and B as "particles" for narrative convenience, they need not be actual particles. All this formalism applies to general subsystems—i.e., subsets of a large quantum system's degrees of freedom. For instance, if a quantum system has a position eigenbasis for 3D space, the x, y, and z coordinates are distinct degrees of freedom, so each position eigenstate is really a tensor product:

$$|\,\mathbf{r} = (x, y, z)\,\rangle \ \equiv \ |x\rangle\,|y\rangle\,|z\rangle. \tag{3.1.10}$$

Also, if the subsystems really *are* particles, we are going to assume for now that the particles are distinguishable. There are other complications that arise if the particles are "identical", which will be the subject of the next chapter (if you're unsure what this means, just read on).

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3.2: Partial Measurements

Let us recall how measurements work in single-particle quantum theory. Each observable Q is described by some Hermitian operator $\hat{Q}$, which has an eigenbasis $\{|q_i\rangle\}$ such that

$$\hat{Q}|q_i\rangle = q_i|q_i\rangle. \tag{3.2.1}$$

For simplicity, let the eigenvalues $\{q_i\}$ be non-degenerate. Suppose a particle initially has quantum state $|\psi\rangle$. This can always be expanded in terms of the eigenbasis of $\hat{Q}$:

$$|\psi\rangle = \sum_i \psi_i\,|q_i\rangle, \quad \text{where} \quad \text{and} \ \ \psi_i = \langle q_i|\psi\rangle. \tag{3.2.2}$$

The **measurement postulate of quantum mechanics** states that if we measure Q, then (i) the probability of obtaining the measurement outcome q_i is $P_i = |\psi_i|^2$, the absolute square of the coefficient of $|q_i\rangle$ in the basis expansion; and (ii) upon obtaining this outcome, the system instantly "collapses" into state $|q_i\rangle$.

Mathematically, these two rules can be summarized using the projection operator

$$\hat{\Pi}(q_i) = |q_i\rangle\langle q_i|. \tag{3.2.3}$$

Applying this operator to $|\psi\rangle$ gives the non-normalized state vector

$$|\psi'\rangle = |q_i\rangle\langle q_i|\psi\rangle. \tag{3.2.4}$$

From this, we glean two pieces of information:

1. The probability of obtaining this outcome is $\langle\psi'|\psi'\rangle = |\langle q_i|\psi\rangle|^2$.
2. The post-collapse state is obtained by the re-normalization $|\psi'\rangle \to |q_i\rangle$.

For multi-particle systems, there is a new complication: what if a measurement is performed on just one particle?

Consider a system of two particles A and B, with two-particle Hilbert space $\mathscr{H}_A \otimes \mathscr{H}_B$. We perform a measurement on particle A, corresponding to a Hermitian operator $\hat{Q}_A$ that acts upon $\mathscr{H}_A$ and has eigenvectors $\{|\mu\rangle \mid \mu = 1, 2, \ldots\}$ (i.e., the eigenvectors are enumerated by some index μ). We can write any state $|\psi\rangle$ using the eigenbasis of $\hat{Q}_A$ for the $\mathscr{H}_A$ part, and an arbitrary basis $\{|\nu\rangle\}$ for the $\mathscr{H}_B$ part:

$$\begin{aligned} |\psi\rangle &= \sum_{\mu\nu} \psi_{\mu\nu}\,|\mu\rangle|\nu\rangle \\ &= \sum_{\mu} |\mu\rangle|\varphi_\mu\rangle, \quad \text{where} \quad |\varphi_\mu\rangle \equiv \sum_\nu \psi_{\mu\nu}\,|\nu\rangle \ \in \ \mathscr{H}_B. \end{aligned} \tag{3.2.5}$$

Unlike the single-particle case, the "coefficient" of $|\mu_i\rangle$ in this basis expansion is not a complex number, but a vector in $\mathscr{H}_B$.

Proceeding by analogy, the probability of obtaining the outcome labelled by μ should be the "absolute square" of this "coefficient", $\langle\varphi_\mu|\varphi_\mu\rangle$. Let us define the partial projector

$$\hat{\Pi}(\mu) \ = \ |\mu\rangle\langle\mu| \otimes \hat{I}\,. \tag{3.2.6}$$

The A slot of this operator contains a projector, $|\mu\rangle\langle\mu|$, while the B slot leaves the $\mathscr{H}_B$ part of the two-particle space unchanged. Applying the partial projector to the state given in Equation (3.2.5) gives

$$|\psi'\rangle \ = \ \hat{\Pi}(\mu)\,|\psi\rangle \ = \ |\mu\rangle|\varphi_\mu\rangle. \tag{3.2.7}$$

Now we follow the same measurement rules as before. The outcome probability is

$$P_\mu = \langle\psi'|\psi'\rangle = \langle\mu|\mu\rangle\,\langle\varphi_\mu|\varphi_\mu\rangle = \sum_\nu |\psi_{\mu\nu}|^2. \tag{3.2.8}$$

The post-measurement collapsed state is obtained by the re-normalization

$$|\psi'\rangle \;\rightarrow\; \frac{1}{\sqrt{\sum_{\nu'}|\psi_{\mu\nu'}|^2}}\sum_{\nu}\psi_{\mu\nu}|\mu\rangle|\nu\rangle. \tag{3.2.9}$$

Example 3.2.1

A system of two spin-$1/2$ particles is in the "singlet state"

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big). \tag{3.2.10}$$

For each particle, $|+z\rangle$ and $|-z\rangle$ denote eigenstates of the operator $\hat{S}_z$, with eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively. Suppose we measure S_z on particle A. What are the probabilities of the possible outcomes, and the associated post-collapse states?

- **First outcome: $+\hbar/2$.**
  - The partial projector is $|+z\rangle\langle+z|\otimes\hat{I}$.
  - Applying the projection to $|\psi\rangle$ yields $|\psi'\rangle = (1/\sqrt{2})\,|+z\rangle|-z\rangle$.
  - The outcome probability is $P_+ = \langle\psi'|\psi'\rangle = \dfrac{1}{2}$.
  - The post-collapse state is $\dfrac{1}{\sqrt{P_+}}|\psi'\rangle = |+z\rangle|-z\rangle$
- **Second outcome: $-\hbar/2$.**
  - The partial projector is $|-z\rangle\langle-z|\otimes\hat{I}$.
  - Applying the projection to $|\psi\rangle$ yields $|\psi'\rangle = (1/\sqrt{2})\,|-z\rangle|+z\rangle$.
  - The outcome probability is $P_- = \langle\psi'|\psi'\rangle = \dfrac{1}{2}$.
  - The post-collapse state is $= \dfrac{1}{\sqrt{P_-}}|\psi'\rangle = |-z\rangle|+z\rangle$.

The two possible outcomes, $+\hbar/2$ and $-\hbar/2$, occur with equal probability. In either case, the two-particle state collapses so that A is in the observed spin eigenstate, and B has the opposite spin. After the collapse, the two-particle state is no longer entangled.

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3.3: The Einstein-Podolsky-Rosen "Paradox"

In 1935, Einstein, Podolsky, and Rosen (EPR) formulated a thought experiment, now known as the **EPR paradox**, that highlights the counter-intuitive features of quantum entanglement. They tried to use this thought experiment to argue that quantum theory cannot serve as a fundamental description of reality. Subsequently, however, it was shown that the EPR paradox is not an actual paradox; physical systems *really do* have the strange behavior that the thought experiment highlighted.

Consider an entangled state, like the following "singlet state" of two spin-$1/2$ particles:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big). \tag{3.3.1}$$

As before, let the two particles be labeled A and B. Measuring S_z on A collapses the system into a two-particle state that is unentangled, where each particle has a definite spin. If the measurement outcome is $+\hbar/2$, the new state is $|+z\rangle|-z\rangle$, whereas if the outcome is $-\hbar/2$, the new state is $|-z\rangle|+z\rangle$.

The postulates of quantum theory seem to indicate that the state collapse happens instantaneously, regardless of the distance separating the particles. Imagine that we prepare the two-particle state in a laboratory on Earth. Particle A is then transported to the laboratory of Alice, in the Alpha Centauri star system, and particle B is transported to the laboratory of Bob, in the Betelgeuse system, separated by ~ 640 light years. In principle, this can be done carefully enough to avoid disturbing the two-particle quantum state.

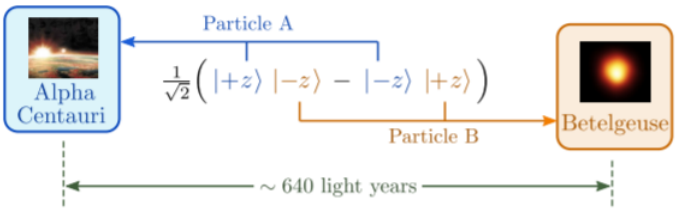

Figure 3.3.1

Once ready, Alice measures $\hat{S}_z$ on particle A, which induces an instantaneous collapse of the two-particle state. Immediately afterwards, Bob measures $\hat{S}_z$ on particle B, and obtains—with 100% certainty—the opposite spin. During the time interval between these two measurements, no classical signal could have traveled between the two star systems, not even at the speed of light. Yet the state collapse induced by Alice's measurement has a definite effect on the result of Bob's measurement.

There are three noteworthy aspects of this phenomenon:

First, it dispels some commonsensical but mistaken "explanations" for quantum state collapse in terms of perturbative effects. For instance, it is sometimes explained that if we want to measure a particle's position, we need to shine a light beam on it, or disturb it in some way, and this disturbance generates an uncertainty in the particle's momentum. The EPR paradox shows that such stories don't capture the full weirdness of quantum state collapse, for we can collapse the state of a particle by doing a measurement on *another* particle far away!

Second, our experimentalists have a certain amount of control over the state collapse, due to the choice of what measurement to perform. So far, we have considered S_z measurements performed by Alice on particle A. But Alice can choose to measure the spin of A along another axis, say S_x. In the basis of spin-up and spin-down states, the operator $\hat{S}_x$ has matrix representation

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.3.2}$$

The eigenvalues and eigenvectors are

$$\begin{aligned} s_x &= \frac{\hbar}{2}, \quad |+x\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle + |-z\rangle\Big) \\ s_x &= -\frac{\hbar}{2}, \quad |-x\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle - |-z\rangle\Big). \end{aligned} \tag{3.3.3}$$

Conversely, we can write the $\hat{S}_z$ eigenstates in the $\{|+x\rangle, |-x\rangle\}$ basis:

$$
\begin{aligned}
|+z\rangle &= \frac{1}{\sqrt{2}}\Big(|+x\rangle + |-x\rangle\Big) \\
|-z\rangle &= \frac{1}{\sqrt{2}}\Big(|+x\rangle - |-x\rangle\Big).
\end{aligned}
\tag{3.3.4}
$$

This allows us to write the two-particle entangled state in the $\hat{S}_x$ basis:

$$
|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|-x\rangle|+x\rangle \; - \; |+x\rangle|-x\rangle\Big). \tag{3.3.5}
$$

Alice's measurement still collapses the particles into definite spin states with opposite spins—but now spin states of S_x rather than S_z.

Third, this ability to choose the measurement axis *does not* allow for superluminal communication. Alice can choose whether to (i) measure S_z or (ii) measure S_x, and this choice instantaneously affects the quantum state of particle B. If Bob can find a way to distinguish between the cases (i) and (ii), even statistically, this would serve as a method for instantaneous communication, violating the theory of relativity! Yet this turns out to be impossible. The key problem is that quantum states themselves cannot be measured; only observables can be measured. Suppose Alice's measurement is $\hat{S}_z$, which collapses B to either $|+z\rangle$ or $|-z\rangle$, each with probability $1/2$. Bob must now choose which measurement to perform. If he measures S_z, the outcome is $+\hbar/2$ or $-\hbar/2$ with equal probabilities. If he measures S_x, the probabilities are:

$$
\begin{aligned}
P(S_x = +\hbar/2) &= \frac{1}{2}\Big|\langle +x|+z\rangle\Big|^2 \; + \; \frac{1}{2}\Big|\langle +x|-z\rangle\Big|^2 = \frac{1}{2} \\
P(S_x = -\hbar/2) &= \frac{1}{2}\Big|\langle -x|+z\rangle\Big|^2 \; + \; \frac{1}{2}\Big|\langle -x|-z\rangle\Big|^2 = \frac{1}{2}.
\end{aligned}
\tag{3.3.6}
$$

The probabilities are still equal! Repeating this analysis for any other choice of spin axis, we find that the two possible outcomes always have equal probability. Thus, Bob's measurement does not yield any information about Alice's choice of measurement axis.

Since quantum state collapse does not allow for superluminal communication, it is consistent *in practice* with the theory of relativity. However, state collapse is still **nonlocal**, in the sense that unobservable ingredients of the theory (quantum states) can change faster than light can travel between two points. For this reason, EPR argued that quantum theory is *philosophically* inconsistent with relativity.

EPR suggested an alternative: maybe quantum mechanics is an approximation of some deeper theory, whose details are currently unknown, but which is deterministic and local. Such a "**hidden variable theory**" may give the appearance of quantum state collapse in the following way. Suppose each particle has a definite but "hidden" value of S_z, either $S_z = +\hbar/2$ or $S_z = -\hbar/2$; let us denote these as $[+]$ or $[-]$. We can hypothesize that the two-particle quantum state $|\psi\rangle$ is not an actual description of reality; rather, it corresponds to a *statistical* distribution of "hidden variable" states, denoted by $[+;-]$ (i.e., $S_z = +\hbar/2$ for particle A and $S_z = -\hbar/2$ for particle B), and $[-;+]$ (the other way around).

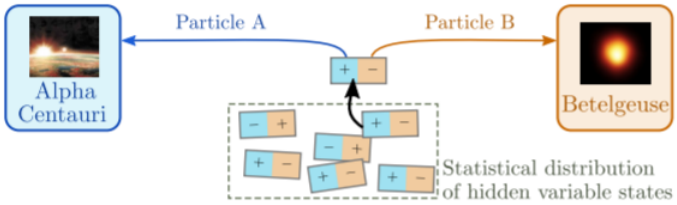

Figure 3.3.2

When Alice measures S_z, the value of the hidden variable is revealed. A result of $+z$ implies $[+;-]$, whereas $-z$ implies $[-;+]$. When bob subsequently measures S_z, the result obtained is the opposite of Alice's result. But those were simply the values all along—there is no instantaneous physical influence traveling between their two laboratories.

Clearly, there are many missing details in this hypothetical description. Any actual hidden variable theory would also need to replicate the huge list of successful predictions made by quantum theory. Trying to come up with a suitable theory of this sort seems difficult, but with enough hard work, one might imagine that it is doable.

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3.4: Bell's Theorem

In 1964, John S. Bell published a bombshell paper showing that the predictions of quantum theory are *inherently inconsistent* with hidden variable theories. The amazing thing about this result, known as **Bell's theorem**, is that it requires no knowledge about the details of the hidden variable theory, just that it is deterministic and local. Here, we present a simplified version of Bell's theorem due to Mermin (1981).

We again consider spin-1/2 particle pairs, with particle A sent to Alice at Alpha Centauri, and particle B to Bob at Betelgeuse. Each experimentalist can measure the particle's spin along three distinct choices of spin axis. These spin observables are denoted by S_1, S_2, and S_3. We will not specify the actual directions of these spin axes until later in the proof. For now, just note that the axes need not correspond to orthogonal spatial directions.

We repeatedly prepare the particle pairs in the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big), \tag{3.4.1}$$

and send the respective particles to Alice and Bob. During each round of the experiment, each experimentalist randomly chooses one of the three spin axes S_1, S_2, or S_3, and performs that spin measurement. It doesn't matter which experimentalist performs the measurement first; the experimentalists can't influence each other, as there is not enough time for a light-speed signal to travel between the two locations. Many rounds of the experiment are conducted; for each round, both experimentalists' choices of spin axis are recorded, along with their measurement results.

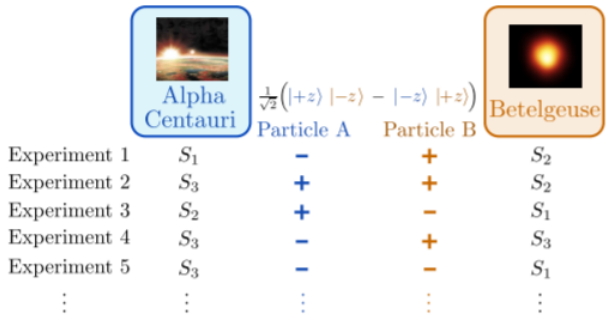
Alpha Centauri
$\frac{1}{\sqrt{2}}\big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\big)$
Particle A
Particle B
Betelgeuse
Experiment 1 S_1 − + S_2
Experiment 2 S_3 + + S_2
Experiment 3 S_2 + − S_1
Experiment 4 S_3 − + S_3
Experiment 5 S_3 − − S_1
⋮ ⋮ ⋮ ⋮ ⋮

Figure 3.4.1

At the end, the experimental records are brought together and examined. We assume that the results are consistent with the predictions of quantum theory. Among other things, this means that whenever the experimentalists happen to choose the same measurement axis, they always find opposite spins. (For example, this is the case during "Experiment 4" in the above figure, where both experimentalists happened to measure S_3.)

Can a hidden variable theory reproduce the results predicted by quantum theory? In a hidden variable theory, each particle must have a definite value for each spin observable. For example, particle A might have $S_1 = +\hbar/2$, $S_2 = +\hbar/2$, $S_3 = -\hbar/2$. Let us denote this by $[++-]$. To be consistent with the predictions of quantum theory, the hidden spin variables for the two particles must have opposite values along each direction. This means that there are 8 distinct possibilities, which we can denote as

$$[+++;---], \quad [++-;--+], \quad [+-+;-+-], \quad [+--;-++],$$
$$[-++;+--], \quad [-+-;+-+], \quad [--+;++-], \quad [---;+++].$$

For instance, $[++-;--+]$ indicates that for particle A, $S_1 = S_2 = +\hbar/2$ and $S_3 = -\hbar/2$, while particle B has the opposite spin values, $S_1 = S_2 = -\hbar/2$ and $S_3 = +\hbar/2$. So far, however, we don't know anything about the relative probabilities of these 8 cases.

Let's now focus on the subset of experiments in which the two experimentalists happened to choose *different* spin axes (e.g., Alice chose S_1 and Bob chose S_2). Within this subset, what is the probability *for the two measurement results to have opposite signs* (i.e., one $+$ and one $-$)? To answer this question, we first look at the following 6 cases:

$$[++-;--+], \quad [+-+;-+-], \quad [+--;-++],$$
$$[-++;+--], \quad [-+-;+-+], \quad [--+;++-].$$

These are the cases which do not have all $+$ or all $-$ for each particle. Consider one of these, say $[++-;--+]$. The two experimentalists picked their measurement axes at random each time, and amongst the experiments where they picked different axes, there are two ways for the measurement results to have opposite signs: (S_1, S_2) or (S_2, S_1). There are four ways to get the same sign: (S_1, S_3), (S_2, S_3), (S_3, S_1) and (S_3, S_2). Thus, for this particular set of hidden variables, the probability for measurement results with opposite signs is 1/3. If we go through all 6 of the cases listed above, we find that in call cases, the probability for opposite signs is 1/3.

Now look at the remaining 2 cases:

$$[+++;---], \quad [---;+++]. \tag{3.4.2}$$

For these, Alice and Bob always obtain results with opposite signs. Combining this with the findings from the previous paragraph, we obtain the following statement:

> *Given that the two experimentalists choose different spin axes, the probability that their results have opposite signs is* $P \geq 1/3$.

This is called **Bell's inequality**. If we can arrange a situation where quantum theory predicts a probability $P < 1/3$ (i.e., a violation of Bell's inequality), that would mean that quantum theory is inherently inconsistent with local deterministic hidden variables. This conclusion would hold regardless of the "inner workings" of the hidden variable theory. In particular, note that the above derivation made no assumptions about the relative probabilities of the hidden variable states.

To complete the proof, we must find a set $\{S_1, S_2, S_3\}$ such that the predictions of quantum mechanics violate Bell's inequality. One simple choice is to align S_1 with the z axis, and align S_2 and S_3 along the x-z plane at 120° ($2\pi/3$ radians) from S_1, as shown below:

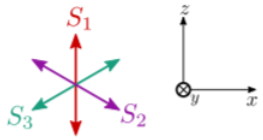

Figure 3.4.2

The corresponding spin operators can be written in the eigenbasis of $\hat{S}_z$:

$$\begin{aligned} \hat{S}_1 &= \frac{\hbar}{2}\sigma_3 \\ \hat{S}_2 &= \frac{\hbar}{2}\left[\cos(2\pi/3)\sigma_3 + \sin(2\pi/3)\sigma_1\right] \\ \hat{S}_3 &= \frac{\hbar}{2}\left[\cos(2\pi/3)\sigma_3 - \sin(2\pi/3)\sigma_1\right]. \end{aligned} \tag{3.4.3}$$

Suppose Alice chooses S_1, and obtains $+\hbar/2$. Particle A collapses to state $|+z\rangle$, and particle B collapses to state $|-z\rangle$. Bob is assumed to choose a different spin axis. If the choice is S_2, the expectation value is

$$\begin{aligned} \langle -z|\, S_2 \,|-z\rangle &= \frac{\hbar}{2}\Big[\cos(2\pi/3)\langle -z|\sigma_3|-z\rangle + \sin(2\pi/3)\langle -z|\sigma_1|-z\rangle\Big] \\ &= \frac{\hbar}{2}\cdot\frac{1}{2} \end{aligned} \tag{3.4.4}$$

If P_+ and P_- respectively denote the probability of measuring $+\hbar/2$ and $-\hbar/2$ in this measurement, the above equation implies that $P_+ - P_- = +1/2$. Moreover, $P_+ + P_- = 1$ by probability conservation. Hence, the probability of obtaining a negative value (the opposite sign from Alice's measurement) is $P_- = 1/4$. All the other possible scenarios are worked out similarly. The result is that the overall probability of the two experimentalists obtaining opposite results (in the cases where they choose different measurement axis) is $1/4$. Bell's inequality is violated!

Last of all, we must consult Nature itself. Is it possible to observe, in an actual experiment, probabilities that violate Bell's inequality? In the decades following Bell's 1964 paper, many experiments were performed to answer this question. These experiments are all substantially more complicated than the simple two-particle spin-$1/2$ model that we've studied, and they are subject to various uncertainties and "loopholes" that are beyond the scope of our discussion. But in the end, the experimental

consensus appears to be a clear *yes*: Nature really does behave according to quantum mechanics, and in a manner that cannot be replicated by deterministic local hidden variables! A summary of the experimental evidence is given in a review paper by Aspect (1999).

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3.5: Quantum Cryptogaphy

One of the most remarkable consequences of Bell's thought experiment is that it provides a way to perform cryptography that is more secure, in certain respects, than conventional cryptography. This possibility was first raised by Ekert, and it has led to a huge amount of research into **quantum cryptography**, which is poised to be one of the most important technological applications of quantum mechanics.

Ekert's quantum cryptography scheme allows two participants, Alice and Bob, to share with each other a string of random binary digits (0 or 1), called a "key", in such a manner that no one else can learn the key by eavesdropping on their communications. Once Alice and Bob have established a secret shared key, it can be used to encrypt subsequent messages between them, which nobody else can decipher (e.g., by using one-time pads).

The scheme follows almost immediately from the Bell thought experiment of Section 3.4. In each round, a pair of spin-$1/2$ particles is prepared in the singlet state, with particle A sent to Alice and B sent to Bob. Alice and Bob each randomly choose a measurement axis (S_1, S_2, or S_3), and measure the spin of their particle along that axis.

After an appropriate number of rounds, Alice and Bob publicly announce their choices of measurement axes. These announcements are assumed to take place over a classical communication channel that cannot be jammed or manipulated by any hostile party (though it can be eavesdropped upon). From the announcements, Alice and Bob determine the rounds in which they happened to pick the same axes. Their measurement results during these rounds are guaranteed to be the opposites of each other. Hence, they have established a random binary string known to each other but to no one else.

How might an eavesdropper, Eve, attempt to foil this scheme? Suppose Eve can intercept some or all of the particles B destined for Bob. She might try to substitute her own measurements, in a manner that could let her work out the secret key. However, Eve is hampered by the fact that she is unable to predict or influence Bob's choices of measurement axes (i.e., Bob's choices are truly random), nor is she able to impersonate Bob during the announcements of the axis choices (i.e., the classical communication channel is unjammable). Under these assumptions, it can be shown that any attempt by Eve to substitute her own measurements can be detected by Alice and Bob, by performing a statistical analysis of their measurement results in the rounds with different different axis choices. The detection of the eavesdropper turns out to be essentially the same as checking for Bell's inequality. For details, refer to Ref.

Alternatively, Eve might try to "clone" the quantum state of particle B before passing it along to Bob. If this can be done, Eve can retain the cloned quantum state, wait for Bob to announce his choice of measurement axis for that round, and then perform the corresponding measurement to reproduce Bob's result. Though plausible at first glance, this turns out to be fundamentally unworkable, as it is incompatible with the laws of quantum mechanics.

The so-called **no-cloning theorem** can be proven as follows. Eve desires to clone an arbitrary state of a spin-half particle B onto another spin-half particle C. The two-particle Hilbert space is $\mathscr{H} \otimes \mathscr{H}$. With particle C initially prepared in some state $|0\rangle$, Eve must devise a unitary operation $\hat{U}$, representing the cloning process, such that

$$\hat{U}|\psi\rangle|0\rangle = e^{i\phi}|\psi\rangle|\psi\rangle \tag{3.5.1}$$

for all $|\psi\rangle \in \mathscr{H}$, and for some phase factor ϕ that could depend on $|\psi\rangle$. Note that the value of ϕ does not affect the outcomes of measurements.

Now replace $|\psi\rangle$ in the above equation with two arbitrary states denoted by $|\psi_1\rangle$ and $|\psi_2\rangle$, and take their inner product. According to Equation (3.5.1),

$$\begin{aligned}\Big(\langle\psi_1|\langle 0|\hat{U}^\dagger\Big)\Big(\hat{U}|\psi_2\rangle|0\rangle\Big) &= \Big(\langle\psi_1|\langle\psi_1|e^{-i\phi_1}\Big)\Big(e^{i\phi_2}|\psi_2\rangle|\psi_2\rangle\Big) \\ &= e^{-i(\phi_1-\phi_2)}\Big(\langle\psi_1|\psi_2\rangle\Big)^2.\end{aligned} \tag{3.5.2}$$

Here, ϕ_1 and ϕ_2 are the phase factors from Equation (3.5.1) for the two chosen states. On the other hand, since $\hat{U}$ is unitary,

$$\begin{aligned}\langle\psi_1|\langle 0|\hat{U}^\dagger\hat{U}|\psi_2\rangle|0\rangle &= \Big(\langle\psi_1|\langle 0|\Big)\Big(|\psi_2\rangle|0\rangle\Big) \\ &= \langle\psi_1|\psi_2\rangle.\end{aligned} \tag{3.5.3}$$

Here we have used the fact that $\langle 0|0\rangle = 1$. Comparing the magnitudes of (3.5.2) and (3.5.3),

$$\left|\langle\psi_1|\psi_2\rangle\right|^2 = \left|\langle\psi_1|\psi_2\rangle\right| \;\;\Rightarrow\;\; \left|\langle\psi_1|\psi_2\rangle\right| = 0 \text{ or } 1. \tag{3.5.4}$$

But aside from the trivial case of a one-dimensional Hilbert space, this cannot be true for arbitrary $|\psi_1\rangle$ and $|\psi_2\rangle$. For instance, for a two-dimensional space spanned by an orthonormal basis $\{|0\rangle, |1\rangle\}$, we can pick

$$|\psi_1\rangle = |0\rangle,\;\; |\psi_2\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle + |1\rangle\big) \;\;\Rightarrow\;\; \left|\langle\psi_1|\psi_2\rangle\right| = \frac{1}{\sqrt{2}}. \tag{3.5.5}$$

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3.6: Density Operators

We now introduce the **density operator**, which helps to streamline many calculations in multi-particle quantum mechanics.

Consider a quantum system with a d-dimensional Hilbert space $\mathscr{H}$. Given an arbitrary state $|\psi\rangle \in \mathscr{H}$, define

$$\hat{\rho} = |\psi\rangle\,\langle\psi|. \tag{3.6.1}$$

This is just the projection operator for $|\psi\rangle$, but in this context we call it a "density operator". Some other authors call it a **density matrix**, based on the fact that linear operators can be represented as matrices. It has the following noteworthy features:

1. It is Hermitian.
2. Suppose $\hat{Q}$ is an observable with eigenvalues $\{q_\mu\}$ and eigenstates $\{|\mu\rangle\}$ (where μ is some label that enumerates the eigenstates. If we do a $\hat{Q}$ measurement on $|\psi\rangle$, the probability of obtaining q_μ is
$$P_\mu = \big|\langle\mu|\psi\rangle\big|^2 = \langle\mu|\,\hat{\rho}\,|\mu\rangle. \tag{3.6.2}$$
3. Moreover, the expectation value of the observable is
$$\langle Q\rangle = \sum_\mu q_\mu P_\mu = \sum_\mu q_\mu \langle\mu|\hat{\rho}|\mu\rangle = \mathrm{Tr}\big[\,\hat{Q}\,\hat{\rho}\,\big]. \tag{3.6.3}$$
In the last equality, $\mathrm{Tr}[\cdots]$ denotes the trace, which is the sum of the diagonal elements of the matrix representation of the operator. The value of the trace is basis-independent.

Now consider, once again, a composite system consisting of two subsystems A and B, with Hilbert spaces $\mathscr{H}_A$ and $\mathscr{H}_B$. Let's say we are interested in the physical behavior of A, that is to say the outcome probabilities and expectation values of any measurements performed on A. These can be calculated from $|\psi\rangle$, the state of the combined system; however, $|\psi\rangle$ also carries information about B, which is not relevant to us as we only care about A.

There is a more economical way to encode just the information about A. We can define the density operator for subsystem A (sometimes called the **reduced density operator**):

$$\hat{\rho}_A = \mathrm{Tr}_B\,\big[\,\hat{\rho}\,\big]. \tag{3.6.4}$$

Here, $\mathrm{Tr}_B[\cdots]$ refers to a **partial trace**. This means tracing over the $\mathscr{H}_B$ part of the Hilbert space $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$, which yields an operator acting on $\mathscr{H}_A$.

To better understand Equation (3.6.4), let us go to an explicit basis. Let $\hat{Q}_A$ be an observable for $\mathscr{H}_A$ with eigenbasis $\{|\mu\rangle\}$, and let $\hat{Q}_B$ be an observable for $\mathscr{H}_B$ with eigenbasis $\{|\nu\rangle\}$. If the density operator of the combined system is $\hat{\rho} = |\psi\rangle\langle\psi|$, then

$$\hat{\rho}_A = \sum_\nu \Big(\hat{I}\otimes\langle\nu|\Big)\;|\psi\rangle\langle\psi|\;\Big(\hat{I}\otimes|\nu\rangle\Big). \tag{3.6.5}$$

This is a Hermitian operator acting on the $\mathscr{H}_A$ space. In the $\{|\mu\rangle\}$ basis, its diagonal matrix elements are

$$\begin{aligned}\langle\mu|\hat{\rho}_A|\mu\rangle &= \sum_\nu \Big(\langle\mu|\langle\nu|\Big)\;|\psi\rangle\langle\psi|\;\Big(|\mu\rangle|\nu\rangle\Big)\\ &= \langle\psi|\;\left[|\mu\rangle\langle\mu|\otimes\left(\sum_\nu |\nu\rangle\langle\nu|\right)\right]\;|\psi\rangle\\ &= \langle\psi|\;\Big(|\mu\rangle\langle\mu|\otimes\hat{I}_B\Big)|\psi\rangle.\end{aligned} \tag{3.6.6}$$

According to the rules of partial measurements discussed in Section 3.2, this is precisely the probability of obtaining q_μ when measuring $\hat{Q}_A$ on subsystem A:

$$P_\mu = \langle\mu|\hat{\rho}_A|\mu\rangle. \tag{3.6.7}$$

It follows that the expectation value for observable $\hat{M}$ is

$$\langle Q_A \rangle = \sum_\mu q_\mu \langle \mu | \hat{\rho}_A | \mu \rangle = \mathrm{Tr}\Big[\hat{Q}_A\, \hat{\rho}_A\Big]. \tag{3.6.8}$$

These results hold for any choice of basis. Hence, knowing the density operator for A, we can determine the outcome probabilities of *any* partial measurement performed on A.

To better understand the properties of $\hat{\rho}_A$, let us write $|\psi\rangle$ explicitly as

$$|\psi\rangle = \sum_{\mu\nu} \psi_{\mu\nu} |\mu\rangle |\nu\rangle, \tag{3.6.9}$$

where $\sum_{\mu\nu} |\psi_{\mu\nu}|^2 = 1$. Then

$$\begin{aligned}
\hat{\rho} &= \sum_{\mu\mu'\nu\nu'} \psi_{\mu\nu}\psi^*_{\mu'\nu'}\ |\mu\rangle|\nu\rangle\,\langle\mu'|\langle\nu'| \\
\hat{\rho}_A &= \sum_{\mu\mu'\nu} \psi_{\mu\nu}\psi^*_{\mu'\nu} |\mu\rangle\langle\mu'| \\
&= \sum_\nu \left(\sum_\mu \psi_{\mu\nu}|\mu\rangle\right)\left(\sum_{\mu'} \psi^*_{\mu'\nu}\langle\mu'|\right) \\
&= \sum_\nu |\varphi_\nu\rangle\langle\varphi_\nu|, \quad \text{where} \quad |\varphi_\nu\rangle = \sum_\mu \psi_{\mu\nu}|\mu\rangle.
\end{aligned} \tag{3.6.10}$$

But $|\varphi_\nu\rangle$ is not necessarily normalized to unity: $\langle\varphi_\nu|\varphi_\nu\rangle = \sum_\mu |\psi_{\mu\nu}|^2 \le 1$. Let us define

$$|\tilde{\varphi}_\nu\rangle = \frac{1}{\sqrt{P_\nu}}|\varphi_\nu\rangle, \quad \text{where} \quad P_\nu = \sum_\mu |\psi_{\mu\nu}|^2. \tag{3.6.11}$$

Note that each P_ν is a non-negative real number in the range $[0, 1]$. Then

$$\hat{\rho}_A = \sum_\nu P_\nu\, |\tilde{\varphi}_\nu\rangle\langle\tilde{\varphi}_\nu|, \quad \text{where} \quad \left\{ \begin{array}{l} \text{each } P_\nu \text{ is a real number in } [0,1], \text{ and} \\ \text{each } |\tilde{\varphi}_\nu\rangle \in \mathscr{H}_A, \ \text{ with } \ \langle\tilde{\varphi}_\nu|\tilde{\varphi}_\nu\rangle = 1. \end{array} \right. \tag{3.6.12}$$

In general, we can define a density operator as any operator that has the form of Equation (3.6.12), regardless of whether or not it was formally derived via a partial trace. We can interpret it as describing a ensemble of quantum states weighted by a set of classical probabilities. Each term in the sum consists of (i) a weighting coefficient P_ν which can be regarded as a probability (the coefficients are all real numbers in the range $[0, 1]$, and sum to 1), and (ii) a projection operator associated with some normalized state vector $|\tilde{\varphi}_\nu\rangle$. Note that the states in the ensemble do not have to be orthogonal to each other.

From this point of view, a density operator of the form $|\psi\rangle\langle\psi|$ corresponds to the special case of an ensemble containing only one quantum state $|\psi\rangle$. Such an ensemble is called a **pure state**, and describes a quantum system that is not entangled with any other system. If an ensemble is not a pure state, we call it a **mixed state**; it describes a system that is entangled with some other system.

We can show that any linear operator $\hat{\rho}_A$ obeying Equation (3.6.12) has the following properties:

1. $\hat{\rho}_A$ is Hermitian.
2. $\langle\varphi|\hat{\rho}_A|\varphi\rangle \ge 0$ for any $|\varphi\rangle \in \mathscr{H}_A$ (i.e., the operator is positive semidefinite).
3. For any observable $\hat{Q}_A$ acting on $\mathscr{H}_A$,

$$\begin{aligned}
\langle Q_A \rangle &\equiv \sum_\nu P_\nu \langle\tilde{\varphi}_\nu|\hat{Q}_A|\tilde{\varphi}_\nu\rangle \\
&= \sum_{\mu\nu} P_\nu\, \langle\tilde{\varphi}_\nu|\mu\rangle\, \langle\mu|\hat{Q}|\tilde{\varphi}_\nu\rangle \quad \big(\text{using some basis } \{|\mu\rangle\}\big) \\
&= \sum_\mu \langle\mu|\hat{Q}\left(\sum_\nu |\tilde{\varphi}_\nu\rangle\langle\tilde{\varphi}_\nu|\right)|\mu\rangle \\
&= \mathrm{Tr}\left[\hat{Q}\,\hat{\rho}_A\right].
\end{aligned} \tag{3.6.13}$$

This property can be used to deduce the probability of obtaining any measurement outcome: if $|\mu\rangle$ is the eigenstate associated with the outcome, the outcome probability is $\langle\mu|\hat{\rho}_A|\mu\rangle$, consistent with Equation (3.6.7). To see this, take $\hat{Q} = |\mu\rangle\langle\mu|$ in Equation (3.6.13).

4. The eigenvalues of $\hat{\rho}_A$, denoted by $\{p_1, p_2, \ldots, p_{d_A}\}$, satisfy

$$p_j \in \mathbb{R} \quad \text{and} \quad 0 \leq p_j \leq 1 \quad \text{for} \quad j = 1, \ldots, d_A, \quad \text{with} \quad \sum_{j=1}^{d_A} p_j = 1. \tag{3.6.14}$$

In other words, the eigenvalues can be interpreted as probabilities. This also implies that $\mathrm{Tr}[\hat{\rho}_A] = 1$.

This property follows from Property 3 by taking $\hat{Q} = |\varphi\rangle\langle\varphi|$, where $|\varphi\rangle$ is any eigenvector of $\hat{\rho}_A$, and then taking $\hat{Q} = \hat{I}_A$.

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3.7: Entanglement Entropy

Previously, we said that a multi-particle system is entangled if the individual particles lack definite quantum states. It would be nice to make this statement more precise, and in fact physicists have come up with several different quantitive measures of entanglement. In this section, we will describe the most common measure, **entanglement entropy**, which is closely related to the entropy concept from thermodynamics, statistical mechanics, and information theory.

We have seen from the previous section that if a subsystem A is (possibly) entangled with some other subsystem B, the information required to calculate all partial measurement outcomes on A is stored within a reduced density operator $\hat{\rho}_A$. We can use this to define a quantity called the **entanglement entropy** of A:

$$S_A = -k_b \,\mathrm{Tr}_A\Big\{\hat{\rho}_A \,\ln\big[\hat{\rho}_A\big]\Big\}. \tag{3.7.1}$$

In this formula, $\ln[\cdots]$ denotes the logarithm of an operator, which is the inverse of the exponential: $\ln(\hat{P}) = \hat{Q} \Rightarrow \exp(\hat{Q}) = \hat{P}$. The prefactor k_b is Boltzmann's constant, and ensures that S_A has the same units as thermodynamic entropy.

The definition of the entanglement entropy is based on an analogy with the entropy concept from classical thermodynamics, statistical mechanics and information theory. In those classical contexts, entropy is a quantitative measure of uncertainty (i.e, lack of information) about a system's underlying microscopic state, or "microstate". Suppose a system has W possible microstates that occur with probabilities $\{p_1, p_2, \ldots, p_W\}$, satisfying $\sum_i p_i = 1$. Then we define the classical entropy

$$S_{\text{cl.}} = -k_b \sum_{i=1}^{W} p_i \ln(p_i). \tag{3.7.2}$$

In a situation of complete certainty where the system is known to be in a specific microstate k ($p_i = \delta_{ik}$), the formula gives $S_{\text{cl.}} = 0$. (Note that $x\ln(x) \to 0$ as $x \to 0$). In a situation of complete uncertainty where all microstates are equally probable ($p_i = 1/W$), we get $S_{\text{cl.}} = k_b \ln W$, the entropy of a microcanonical ensemble in statistical mechanics. For any other distribution of probabilities, it can be shown that the entropy lies between these two extremes: $0 \le S_{\text{cl.}} \le k_b \ln W$. For a review of the properties of entropy, see Appendix C.

The concept of entanglement entropy aims to quantify the uncertainty arising from a quantum (sub)system's lack of a definite quantum state, due to it being possibly entangled with another (sub)system. When formulating it, the key issue we need to be careful about is how to extend classical notions of probability to quantum systems. We have seen that when performing a measurement on A whose possible outcomes are $\{q_\mu\}$, the probability of getting q_μ is $P_\mu = \langle\mu|\hat{\rho}_A|\mu\rangle$. However, it is problematic to directly substitute these probabilities $\{P_\mu\}$ into the classical entropy formula, since they are basis-dependent (i.e., the set of probabilities is dependent on the choice of measurement). Equation (3.7.1) bypasses this problem by using the trace, which is basis-independent.

In the special case where $\{|\mu\rangle\}$ is the eigenbasis for $\hat{\rho}_A$, the connection is easier to see. From (3.7.2), the eigenvalues $\{p_\mu\}$ are all real numbers between 0 and 1, and summing to unity, so they can be regarded as probabilities. Then the entanglement entropy is

$$\begin{aligned} S_A &= -k_b \sum_\mu \langle\mu|\hat{\rho}_A \ln(\hat{\rho}_A)|\mu\rangle \\ &= -k_b \sum_\mu p_\mu \ln(p_\mu). \end{aligned} \tag{3.7.3}$$

Therefore, in this particular basis the expression for the entanglement entropy is consistent with the classical definition of entropy, with the eigenvalues of $\hat{\rho}_A$ serving as the relevant probabilities.

By analogy with the classical entropy formula (see Appendix C), the entanglement entropy has the following bounds:

$$0 \le S_A \le k_b \ln(d_A), \tag{3.7.4}$$

where d_A is the dimension of $\mathscr{H}_A$.

The lower bound $S_A = 0$ holds if and only if system A is in a pure state (i.e., it is not entangled with any other system). This is because the bound corresponds to a situation where $\hat{\rho}_A$ has one eigenvalue that is 1, and all the other eigenvalues are 0 (see Appendix C). If we denote the eigenvector associated with the non-vanishing eigenvalue by $|\psi\rangle$, then the density matrix can be written as $\hat{\rho}_A = |\varphi\rangle\langle\varphi|$, which has the form of a pure state.

As a corollary, if we find that $S_A \neq 0$, then $\hat{\rho}_A$ cannot be written as a pure state $|\psi\rangle\langle\psi|$ for *any* $|\psi\rangle$, and hence it must describe a mixed state.

A system is said to be **maximally entangled** if it saturates the upper bound of (3.7.4), $S_A = k_b \ln(d_A)$. This occurs if and only if the eigenvalues of the density operator are all equal: i.e., $p_j = 1/d_A$ for all $j = 1, \ldots, d_A$.

Example 3.7.1

Consider the following state of two spin-$1/2$ particles:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big). \tag{3.7.5}$$

The density operator for the two-particle system is

$$\hat{\rho}(\psi) = \frac{1}{2}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big)\Big(\langle+z|\langle-z| - \langle-z|\langle+z|\Big). \tag{3.7.6}$$

Tracing over system B (the second slot) yields the reduced density operator

$$\hat{\rho}_A(\psi) = \frac{1}{2}\Big(|+z\rangle\langle+z| + |-z\rangle\langle-z|\Big). \tag{3.7.7}$$

This can be expressed as a matrix in the $\{|+z\rangle, |-z\rangle\}$ basis:

$$\hat{\rho}_A(\psi) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{3.7.8}$$

Now we can use $\hat{\rho}_A$ to compute the entanglement entropy

$$S_A = -k_b \mathrm{Tr}\left\{\hat{\rho}_A \ln(\rho_A)\right\} = -k_b \mathrm{Tr}\begin{pmatrix} \frac{1}{2}\ln\left(\frac{1}{2}\right) & 0 \\ 0 & \frac{1}{2}\ln\left(\frac{1}{2}\right) \end{pmatrix} = k_b \ln(2). \tag{3.7.9}$$

Hence, the particles are maximally entangled.

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3.8: The Many Worlds Interpretation

We conclude this chapter by discussing a set of compelling but controversial ideas arising from the phenomenon of quantum entanglement: the **Many Worlds Interpretation** as formulated by Hugh Everett (1956).

So far, when describing the phenomenon of state collapse, we have relied on the measurement postulate (see Section 3.2), which is part of the **Copenhagen Interpretation** of quantum mechanics. This is how quantum mechanics is typically taught, and how physicists think about the theory when doing practical, everyday calculations.

However, the measurement postulate has two bad features:

1. It stands apart from the other postulates of quantum mechanics, for it is the only place where randomness (or "indeterminism") creeps into quantum theory. The other postulates do not refer to probabilities. In particular, the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \tag{3.8.1}$$

   is completely deterministic. If you know $\hat{H}(t)$ and are given the state $|\psi(t_0)\rangle$ at some time t_0, you can in principle determine $|\psi(t)\rangle$ for all t. This time-evolution consists of a smooth, non-random rotation of the state vector within its Hilbert space. A measurement process, however, has a completely different character: it causes the state vector to jump discontinuously to a randomly-selected value. It is strange that quantum theory contains two completely different ways for a state to change.

2. The measurement postulate is silent on what constitutes a measurement. Does measurement require a conscious observer? Surely not: as Einstein once exasperatedly asked, are we really expected to believe that the Moon exists only when we look at it? But if a given device interacts with a particle, what determines whether it acts via the Schrödinger equation, or performs a measurement?

The Many Worlds Interpretation seeks to resolve these problems by positing that *the measurement postulate is not a fundamental postulate of quantum mechanics.* Rather, what we call "measurement", including state collapse and the apparent randomness of measurement results, is an emergent phenomenon that can be derived from the behavior of complex many-particle quantum systems obeying the Schrödinger equation. The key idea is that a measurement process can be described by applying the Schrödinger equation to a quantum system containing both the thing being measured *and* the measurement apparatus itself.

We can study this using a toy model formulated by Albrecht (1993). Consider a spin-$1/2$ particle, and an apparatus designed to measure S_z. Let $\mathscr{H}_S$ be the spin-$1/2$ Hilbert space (which is 2D), and $\mathscr{H}_A$ be the Hilbert space of the apparatus (which has dimension d). We will assume that d is very large, as actual experimental apparatuses are macroscopic objects containing 10^{23} or more atoms! The Hilbert space of the combined system is

$$\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_A, \tag{3.8.2}$$

and is $2d$-dimensional. Let us suppose the system is prepared in an initial state

$$|\psi(0)\rangle = \Big(a_+|+z\rangle + a_-|-z\rangle\Big) \otimes |\Psi\rangle, \tag{3.8.3}$$

where $a_\pm \in \mathbb{C}$ are the quantum amplitudes for the particle to be initially spin-up or spin-down, and $|\Psi\rangle \in \mathscr{H}_A$ is the initial state of the apparatus.

The combined system now evolves via the Schrödinger equation. We aim to show that if the Hamiltonian has the form

$$\hat{H} = \hat{S}_z \otimes \hat{V}, \tag{3.8.4}$$

where $\hat{S}_z$ is the operator corresponding to the observable S_z, then time evolution has an effect equivalent to the measurement of S_z.

It turns out that we can show this without making any special choices for $\hat{V}$ or $|\Psi\rangle$. We only need $d \gg 2$, and for both $\hat{V}$ and $|\Psi\rangle$ to be "sufficiently complicated". We choose $|\Psi\rangle$ to be a random state vector, and choose random matrix components for the operator $\hat{V}$. The precise generation procedures will be elaborated on later. Once we decide on $|\Psi\rangle$ and $\hat{V}$, we can evolve the system by solving the Schödinger equation

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle, \quad \text{where } \hat{U}(t) = \exp\left[-\frac{i}{\hbar}\hat{H}t\right]. \tag{3.8.5}$$

Because the part of $\hat{H}$ acting on the $\mathscr{H}_S$ subspace is $\hat{S}_z$, the result necessarily has the following form:

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)\Big(a_+|{+z}\rangle + a_-|{-z}\rangle\Big)\otimes|\Psi\rangle \\ &= a_+|{+z}\rangle\otimes|\Psi_+(t)\rangle \;+\; a_-|{-z}\rangle\otimes|\Psi_-(t)\rangle. \end{aligned} \tag{3.8.6}$$

Here, $|\Psi_+(t)\rangle$ and $|\Psi_-(t)\rangle$ are apparatus states that are "paired up" with the $|{+z}\rangle$ and $|{-z}\rangle$ states of the spin-$1/2$ subsystem. At $t=0$, both $|\Psi_+(t)\rangle$ and $|\Psi_-(t)\rangle$ are equal to $|\Psi\rangle$; for $t>0$, they rotate into different parts of the state space $\mathscr{H}_A$. If the dimensionality of $\mathscr{H}_A$ is sufficiently large, and both $\hat{V}$ and $|\Psi\rangle$ are sufficiently complicated, we can guess (and we will verify numerically) that the two state vectors rotate into completely different parts of the state space, so that

$$\langle\Psi_+(t)|\Psi_-(t)\rangle \approx 0 \quad \text{for sufficiently large } \; t. \tag{3.8.7}$$

Once this is the case, the two terms in the above expression for $|\psi(t)\rangle$ can be interpreted as two decoupled "worlds". In one world, the spin has a definite value $+\hbar/2$, and the apparatus is in a state $|\Psi_+\rangle$ (which might describe, for instance, a macroscopically-sized physical pointer that is pointing to a "$S_z=+\hbar/2$" reading). In the other world, the spin has a definite value $-\hbar/2$, and the apparatus has a different state $|\Psi_-\rangle$ (which might describe a physical pointer pointing to a "$S_z=-\hbar/2$" reading). Importantly, the $|\Psi_+\rangle$ and $|\Psi_-\rangle$ states are orthogonal, so they can be rigorously distinguished from each other. The two worlds are "weighted" by $|a_+|^2$ and $|a_-|^2$, which correspond to the probabilities of the two possible measurement results.

The above description can be tested numerically. Let us use an arbitrary basis for the apparatus space $\mathscr{H}_A$; in that basis, let the d components of the initial apparatus state vector $|\Psi\rangle$ be random complex numbers:

$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{N}}}\begin{pmatrix}\Psi_0\\ \Psi_1\\ \vdots\\ \Psi_{d-1}\end{pmatrix}, \quad \text{where} \;\; \mathrm{Re}(\Psi_j), \mathrm{Im}(\Psi_j) \sim N(0,1).$$

In other words, the real and imaginary parts of each complex number Ψ_j are independently drawn from the the standard normal (Gaussian) distribution, denoted by $N(0,1)$. The normalization constant $\mathcal{N}$ is defined so that $\langle\Psi|\Psi\rangle = 1$.

Likewise, we generate the matrix elements of $\hat{V}$ according to the following random scheme:

$$\begin{aligned} A_{ij} &\sim u_{ij} + i v_{ij}, \quad \text{where} \;\; u_{ij}, v_{ij} \sim N(0,1) \\ \hat{V} &= \frac{1}{2\sqrt{d}}\left(\hat{A} + \hat{A}^\dagger\right). \end{aligned} \tag{3.8.8}$$

This scheme produces a $d\times d$ matrix with random components, subject to the requirement that the overall matrix be Hermitian. The factor of $1/2\sqrt{d}$ is relatively unimportant; it ensures that the eigenvalues of $\hat{V}$ lie in the range $[-2,2]$, instead of scaling with d, see Edelman and Rao (2005).

The Schrödinger equation can now be solved numerically. The results are shown below:

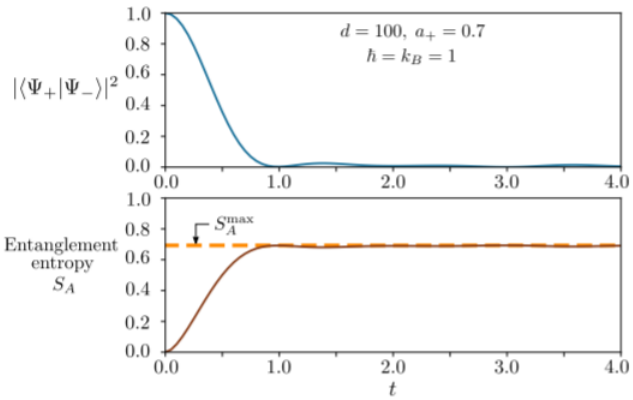

Figure 3.8.1

In the initial state, we let $a_+ = 0.7$, so $a_- = \sqrt{1-0.7^2} = 0.71414\ldots$ The upper panel plots the overlap between the two apparatus states, $|\langle\Psi_+|\Psi_-\rangle|^2$, versus t. In accordance with the preceding discussion, the overlap is unity at $t=0$, but subsequently

decreases to nearly zero. For comparison, the lower panel plots the entanglement entropy between the two subsystems, $S_A = -k_b \mathrm{Tr}_A \{\hat{\rho}_A \ln \hat{\rho}_A\}$, where $\hat{\rho}_A$ is the reduced density matrix obtained by tracing over the spin subspace. We find that $S_A = 0$ at $t = 0$, due to the fact that the spin and apparatus subsystems start out with definite quantum states in $|\psi(0)\rangle$. As the system evolves, the subsystems become increasingly entangled, and S_A increases up to

$$S_A^{\max}/k_b = -\left(|a_+|^2 \ln |a_+|^2 + |a_-|^2 \ln |a_-|^2\right) \approx 0.693 \tag{3.8.9}$$

This value is indicated in the figure by a horizontal dashed line, and corresponds to the result of the classical entropy formula for probabilities $\{|a_+|^2, |a_-|^2\}$. Moreover, we see that the entropy reaches $S_A^{\max}$ at around the same time that $|\langle \Psi_+ | \Psi_- \rangle|^2$ reaches zero. This demonstrates the close relationship between "measurement" and "entanglement".

For details about the numerical linear algebra methods used to perform the above calculation, refer to Appendix D.

The "many worlds" concept can be generalized from the above toy model to the universe as a whole. In the viewpoint of the Many Worlds Interpretation of quantum mechanics, the entire universe can be described by a mind-bogglingly complicated quantum state, evolving deterministically according to the Schrödinger equation. This evolution involves repeated "branchings" of the universal quantum state, which continuously produces more and more worlds. The classical world that we appear to inhabit is just one of a vast multitude. It is up to you to decide whether this conception of reality seems reasonable. It is essentially a matter of preference, because the Copenhangen Interpretation and the Many Worlds Interpretation have identical physical consequences, which is why they are referred to as different "interpretations" of quantum mechanics, rather than different theories.

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3.9: Exercises

Exercises

Exercise 3.9.1

Let $\mathscr{H}_A$ and $\mathscr{H}_B$ denote single-particle Hilbert spaces with well-defined inner products. That is to say, for all vectors $|\mu\rangle, |\mu'\rangle, |\mu''\rangle \in \mathscr{H}_A$, that Hilbert space's inner product satisfies the inner product axioms

a. $\langle\mu|\mu'\rangle = \langle\mu'|\mu\rangle^*$

b. $\langle\mu|\mu\rangle \in \mathbb{R}_0^+$, and $\langle\mu|\mu\rangle = 0$ if and only if $|\mu\rangle = 0$.

c. $\langle\mu|\left(|\mu'\rangle + |\mu''\rangle\right) = \langle\mu|\mu'\rangle + \langle\mu|\mu''\rangle$

d. $\langle\mu|\left(c|\mu'\rangle\right) = c\langle\mu|\mu'\rangle$ for all $c \in \mathbb{C}$,

and likewise for vectors from $\mathscr{H}_B$ with that Hilbert space's inner product.

In Section 3.1, we defined a tensor product space $\mathscr{H}_A \otimes \mathscr{H}_B$ as the space spanned by the basis vectors $\{|\mu\rangle \otimes |\nu\rangle\}$, where the $|\mu\rangle$'s are basis vectors for $\mathscr{H}_A$ and the $|\nu\rangle$'s are basis vectors for $\mathscr{H}_B$. Prove that we can define an inner product using

$$\Big(\langle\mu| \otimes \langle\nu|\Big)\Big(|\mu'\rangle \otimes |\nu'\rangle\Big) \equiv \langle\mu|\mu'\rangle\,\langle\nu|\nu'\rangle = \delta_{\mu\mu'}\delta_{\nu\nu'} \tag{3.9.1}$$

which satisfies the inner product axioms.

Exercise 3.9.2

Consider the density operator

$$\hat{\rho} = \frac{1}{2}|{+z}\rangle\langle{+z}| + \frac{1}{2}|{+x}\rangle\langle{+x}| \tag{3.9.2}$$

where $|{+x}\rangle = \frac{1}{\sqrt{2}}(|{+z}\rangle + |{-z}\rangle)$. This can be viewed as an equal-probability sum of two different pure states. However, the density matrix can also be written as

$$\hat{\rho} = p_1\,|\psi_1\rangle\langle\psi_1| + p_2\,|\psi_2\rangle\langle\psi_2| \tag{3.9.3}$$

where $|\psi_1\rangle$ and $|\psi_2\rangle$ are the eigenvectors of $\hat{\rho}$. Show that p_1 and p_2 are *not* 1/2.

Exercise 3.9.3

Consider two distinguishable particles, A and B. The 2D Hilbert space of A is spanned by $\{|m\rangle, |n\rangle\}$, and the 3D Hilbert space of B is spanned by $\{|p\rangle, |q\rangle, |r\rangle\}$. The two-particle state is

$$|\psi\rangle = \frac{1}{3}\,|m\rangle|p\rangle + \frac{1}{\sqrt{6}}\,|m\rangle|q\rangle + \frac{1}{\sqrt{18}}\,|m\rangle|r\rangle + \frac{\sqrt{2}}{3}\,|n\rangle|p\rangle + \frac{1}{\sqrt{3}}\,|n\rangle|q\rangle + \frac{1}{3}\,|n\rangle|r\rangle. \tag{3.9.4}$$

Find the entanglement entropy.

Further Reading

[1] Bransden & Joachain, §14.1—14.4, §17.1–17.5

[2] Sakurai, §3.9

[3] A. Einstein, B. Podolsky, and N. Rosen, *Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?*, Physical Review **47**, 777 (1935).

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CHAPTER OVERVIEW

4: Identical Particles

These our actors,
As I foretold you, were all spirits and
Are melted into air, into thin air:
And, like the baseless fabric of this vision,
The cloud-capp'd towers, the gorgeous palaces,
The solemn temples, the great globe itself,
Yea, all which it inherit, shall dissolve
And, like this insubstantial pageant faded,
Leave not a rack behind.

William Shakespeare, *The Tempest*

4.1: Particle Exchange Symmetry
4.2: Symmetric and Antisymmetric States
4.3: Second Quantization
4.4: Quantum Field Theory
4.5: Exercises

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4.1: Particle Exchange Symmetry

In the previous chapter, we discussed how the principles of quantum mechanics apply to systems of multiple particles. That discussion omitted an important feature of multi-particle systems, namely the fact that particles of the same type are fundamentally indistinguishable from each other. As it turns out, indistinguishability imposes a strong constraint on the form of the multi-particle quantum states, and looking into this will ultimately lead us to a fundamental re-interpretation of what "particles" are.

Suppose we have two particles of the same type, e.g. two electrons. It is a fact of Nature that all electrons have identical physical properties: the same mass, same charge, same total spin, etc. As a consequence, the single-particle Hilbert spaces of the two electrons must be mathematically identical. Let us denote this space by $\mathscr{H}^{(1)}$. For a two-electron system, the Hilbert space is a tensor product of two single-electron Hilbert spaces, denoted by

$$\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}. \tag{4.1.1}$$

Moreover, any Hamiltonian must affect the two electrons in a symmetrical way. An example of such a Hamiltonian is

$$\hat{H} = \frac{1}{2m_e}\left(|\hat{\mathbf{p}}_1|^2 + |\hat{\mathbf{p}}_2|^2\right) + \frac{e^2}{4\pi\varepsilon_0|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|}, \tag{4.1.2}$$

consisting of the non-relativistic kinetic energies and the Coulomb potential energy. Operators $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{r}}_1$ act on electron 1, while $\hat{\mathbf{p}}_2$ and $\hat{\mathbf{r}}_2$ act on electron 2.

Evidently, this Hamiltonian is invariant under an interchange of the operators acting on the two electrons (i.e., $\hat{\mathbf{p}}_1 \leftrightarrow \hat{\mathbf{p}}_2$ and $\hat{\mathbf{r}}_1 \leftrightarrow \hat{\mathbf{r}}_2$). This can be regarded as a kind of symmetry, called **exchange symmetry**. As we know, symmetries of quantum systems can be represented by unitary operators that commute with the Hamiltonian. Exchange symmetry is represented by an operator $\hat{P}$, defined as follows: let $\{|\mu\rangle\}$ be a basis for the single-electron Hilbert space $\mathscr{H}^{(1)}$; then $\hat{P}$ interchanges the basis vectors for the two electrons:

$$\begin{aligned}\hat{P}\Big(\sum_{\mu\nu}\psi_{\mu\nu}|\mu\rangle|\nu\rangle\Big) \;&\equiv\; \sum_{\mu\nu}\psi_{\mu\nu}|\nu\rangle|\mu\rangle \\ &= \sum_{\mu\nu}\psi_{\nu\mu}|\nu\rangle|\mu\rangle \quad (\text{interchanging } \mu \leftrightarrow \nu \text{ in the double sum})\end{aligned} \tag{4.1.3}$$

The exchange operator has the following properties:

1. $\hat{P}^2 = \hat{I}$, where $\hat{I}$ is the identity operator.
2. $\hat{P}$ is linear, unitary, and Hermitian (see Exercise 4.5.1).
3. The effect of $\hat{P}$ does not depend on the choice of basis (see Exercise 4.5.1).
4. $\hat{P}$ commutes with the above Hamiltonian $\hat{H}$; more generally, it commutes with any two-particle operator built out of symmetrical combinations of single-particle operators (see Exercise 4.5.2).

According to Noether's theorem, any symmetry implies a conservation law. In the case of exchange symmetry, $\hat{P}$ is both Hermitian *and* unitary, so we can take the conserved quantity to be the eigenvalue of $\hat{P}$ itself. We call this eigenvalue, p, the **exchange parity**. Given that $\hat{P}^2 = \hat{I}$, there are just two possibilities:

$$\hat{P}|\psi\rangle = p|\psi\rangle \quad \Rightarrow \quad p = \begin{cases} +1 & (\text{"symmetric state"}), \text{ or} \\ -1 & (\text{"antisymmetric state"}). \end{cases} \tag{4.1.4}$$

Since $\hat{P}$ commutes with $\hat{H}$, if the system starts out in an eigenstate of $\hat{P}$ with parity p, it retains the same parity for all subsequent times.

The concept of exchange parity generalizes to systems of more than two particles. Given N particles, we can define a set of exchange operators $\hat{P}_{ij}$, where $i, j \in \{1, 2, \ldots, N\}$ and $i \neq j$, such that $\hat{P}_{ij}$ exchanges particle i and particle j. If the particles are identical, the Hamiltonian must commute with *all* the exchange operators, so the parities (± 1) are individually conserved.

We now invoke the following postulates:

1. A multi-particle state of identical particles is an eigenstate of every $\hat{P}_{ij}$.

2. For each $\hat{P}_{ij}$, the exchange parity p_{ij} has the same value: i.e., all $+1$ or all -1.
3. The exchange parity p_{ij} is determined solely by the type of particle involved.

Do *not* think of these as statements as being derived from more fundamental facts! Rather, they are hypotheses about the way particles behave—facts about Nature that physicists have managed to deduce through examining a wide assortment of empirical evidence. Our task, for now, shall be to explore the consequences of these hypotheses.

Particles that have symmetric states ($p_{ij} = +1$) are called **bosons**. It turns out that the elementary particles that "carry" the fundamental forces are all bosons: these are the photons (elementary particles of light, which carry the electromagnetic force), gluons (elementary particles that carry the strong nuclear force, responsible for binding protons and neutrons together), and W and Z bosons (particles that carry the weak nuclear force responsible for beta decay). Other bosons include particles that carry non-fundamental forces, such as phonons (particles of sound), as well as certain composite particles such as alpha particles (helium-4 nuclei).

Particles that have antisymmetric states ($p_{ij} = -1$) are called **fermions**. All the elementary particles of "matter" are fermions: electrons, muons, tauons, quarks, neutrinos, and their anti-particles (positrons, anti-neutrinos, etc.). Certain composite particles are also fermions, including protons and neutrons, which are each composed of three quarks.

By the way, one might question whether particle indistinguishability invalidates the concept of assigning single-particle states to (say) the "first slot" or "second slot" in a tensor product. It seems unsatisfactory that our mathematical framework allows us to write down a state like $|\mu\rangle|\nu\rangle$ (where $\mu \neq \nu$), which is physically impossible since it is not symmetric or antisymmetric, and then uses such states to define a "particle exchange" operation that has no physical meaning. To get around this, Leinaas and Myrheim (1977) have developed an interesting formulation of particle indistinguishability that avoids the concept of particle exchange. In this view, in a multi-particle wavefunction the coordinates $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ are not to be regarded as an ordinary vector, but as a mathematical object in which interchanging entries leaves the object invariant. Bosonic or fermionic states can then be constructed by carefully analyzing the topological structure of wavefunctions defined on such configuration spaces. For more details, the interested reader is referred to the paper by Leinaas and Myrheim. In this course, however, we will adopt the usual formulation based on particle exchange.

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4.2: Symmetric and Antisymmetric States

Bosons

A state of N bosons must be symmetric under every possible exchange operator:

$$\hat{P}_{ij}\,|\psi\rangle = |\psi\rangle \quad \forall i,j \in \{1,\ldots,N\}, \quad i \neq j. \tag{4.2.1}$$

There is a standard way to construct multi-particle states obeying this symmetry condition. First, consider a two-boson system ($N = 2$). If both bosons occupy the same single-particle state, $|\mu\rangle \in \mathscr{H}^{(1)}$, the two-boson state is simply

$$|\mu,\mu\rangle = |\mu\rangle|\mu\rangle. \tag{4.2.2}$$

This evidently satisfies the required symmetry condition (4.2.1). Next, suppose the two bosons occupy *different* single-particle states, $|\mu\rangle$ and $|\nu\rangle$, which are orthonormal vectors in $\mathscr{H}^{(1)}$. It would be wrong to write the two-boson state as $|\mu\rangle|\nu\rangle$, because the particles would not be symmetric under exchange. Instead, we construct the multi-particle state

$$|\mu,\nu\rangle = \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle\Big). \tag{4.2.3}$$

This has the appropriate exchange symmetry:

$$\hat{P}_{12}\,|\mu,\nu\rangle \;=\; \frac{1}{\sqrt{2}}\Big(|\nu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle\Big) \;=\; |\mu,\nu\rangle. \tag{4.2.4}$$

The $1/\sqrt{2}$ factor in Equation (4.2.3) ensures that the state is normalized (check for yourself that this is true—it requires $|\mu\rangle$ and $|\nu\rangle$ to be orthonormal to work out).

The above construction can be generalized to arbitrary numbers of bosons. Suppose we have N bosons occupying single-particle states enumerated by

$$|\phi_1\rangle,\ |\phi_2\rangle,\ |\phi_3\rangle,\ \ldots,|\phi_N\rangle. \tag{4.2.5}$$

Each of the states $|\phi_j\rangle$ is drawn from an orthonormal basis set $\{|\mu\rangle\}$ for $\mathscr{H}^{(1)}$. We use the ϕ labels to indicate that the listed states can overlap. For example, we could have $|\phi_1\rangle = |\phi_2\rangle = |\mu\rangle$, meaning that the single-particle state $|\mu\rangle$ is occupied by two particles.

The N-boson state can now be written as

$$|\phi_1,\phi_2,\ldots,\phi_N\rangle = \mathcal{N}\sum_p \Big(|\phi_{p(1)}\rangle|\phi_{p(2)}\rangle|\phi_{p(3)}\rangle\cdots|\phi_{p(N)}\rangle\Big). \tag{4.2.6}$$

The sum is taken over each of the $N!$ permutations acting on $\{1,2,\ldots,N\}$. For each permutation p, we let $p(j)$ denote the integer that j is permuted into.

The prefactor $\mathcal{N}$ is a normalization constant, and it can be shown that its appropriate value is

$$\mathcal{N} = \sqrt{\frac{1}{N!n_a!n_b!\cdots}}, \tag{4.2.7}$$

where n_μ denotes the number of particles in each distinct state $|\varphi_\mu\rangle$, and $N = n_\alpha + n_\beta + \cdots$ is the total number of particles. The proof of this is left as an exercise (Exercise 4.5.3).

To see that the above N-particle state is symmetric under exchange, apply an arbitrary exchange operator $\hat{P}_{ij}$:

$$\begin{aligned}\hat{P}_{ij}|\phi_1,\phi_2,\ldots,\phi_N\rangle &= \mathcal{N}\sum_p \hat{P}_{ij}\Big(\cdots|\phi_{p(i)}\rangle\cdots|\phi_{p(j)}\rangle\cdots\Big)\\ &= \mathcal{N}\sum_p \Big(\cdots|\phi_{p(j)}\rangle\cdots|\phi_{p(i)}\rangle\cdots\Big).\end{aligned} \tag{4.2.8}$$

In each term of the sum, two states i and j are interchanged. Since the sum runs through all permutations of the states, the result is the same with or without the exchange, so we still end up with $|\phi_1,\phi_2,\ldots,\phi_N\rangle$. Therefore, the multi-particle state is symmetric under every possible exchange operation.

Example 4.2.1

A three-boson system has two particles in a state $|\mu\rangle$, and one particle in a different state $|\nu\rangle$. To express the three-particle state, define $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle\}$ where $|\phi_1\rangle = |\phi_2\rangle = |\mu\rangle$ and $|\phi_3\rangle = |\nu\rangle$. Then

$$\begin{aligned} |\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{12}}\Big(|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle + |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle + |\phi_3\rangle|\phi_1\rangle|\phi_2\rangle \\ &\qquad + |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle + |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle + |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle\Big) \\ &= \frac{1}{\sqrt{3}}\Big(|\mu\rangle|\mu\rangle|\nu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle\Big). \end{aligned} \tag{4.2.9}$$

The exchange symmetry operators have the expected effects:

$$\begin{aligned} \hat{P}_{12}|\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}}\Big(|\mu\rangle|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle\Big) = |\phi_1, \phi_2, \phi_3\rangle \\ \hat{P}_{23}|\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}}\Big(|\mu\rangle|\nu\rangle|\mu\rangle + |\mu\rangle|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle\Big) = |\phi_1, \phi_2, \phi_3\rangle \\ \hat{P}_{13}|\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}}\Big(|\nu\rangle|\mu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle + |\mu\rangle|\mu\rangle|\nu\rangle\Big) = |\phi_1, \phi_2, \phi_3\rangle. \end{aligned} \tag{4.2.10}$$

Fermions

A state of N fermions must be antisymmetric under every possible exchange operator:

$$\hat{P}_{ij}\,|\psi\rangle = -|\psi\rangle \quad \forall\, i, j \in \{1, \ldots, N\},\ i \neq j. \tag{4.2.11}$$

Similar to the bosonic case, we can explicitly construct multi-fermion states based on the occupancy of single-particle state.

First consider $N = 2$, with the fermions occupying the single-particle states $|\mu\rangle$ and $|\nu\rangle$ (which, once again, we assume to be orthonormal). The appropriate two-particle state is

$$|\mu, \nu\rangle = \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle - |\nu\rangle|\mu\rangle\Big). \tag{4.2.12}$$

We can easily check that this is antisymmetric:

$$\hat{P}_{12}|\mu, \nu\rangle = \frac{1}{\sqrt{2}}\Big(|\nu\rangle|\mu\rangle - |\mu\rangle|\nu\rangle\Big) = -|\mu, \nu\rangle. \tag{4.2.13}$$

Note that if $|\mu\rangle$ and $|\nu\rangle$ are the same single-particle state, Equation (4.2.12) doesn't work, since the two terms would cancel to give the zero vector, which is not a valid quantum state. This is a manifestation of the **Pauli exclusion principle**, which states that two fermions cannot occupy the same single-particle state. Thus, each single-particle state is either unoccupied or occupied by one fermion.

For general N, let the occupied single-particle states be $|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle$, each drawn from some orthonormal basis $\{|\mu\rangle\}$ for $\mathscr{H}^{(1)}$, and each distinct. Then the appropriate N-fermion state is

$$|\phi_1, \ldots, \phi_N\rangle = \frac{1}{\sqrt{N!}} \sum_p s(p)\, |\phi_{p(1)}\rangle|\phi_{p(2)}\rangle \cdots |\phi_{p(N)}\rangle. \tag{4.2.14}$$

It is up to you to verify that the $1/\sqrt{N!}$ prefactor is the right normalization constant. The sum is taken over every permutation p of the sequence $\{1, 2, \ldots, N\}$, and each term in the sum has a coefficient $s(p)$ denoting the **parity of the permutation**. The parity of any permutation p is defined as $+1$ if p is constructed from an even number of transpositions (i.e., exchanges of adjacent elements) starting from the sequence $\{1, 2, \ldots, N\}$, and -1 if p involves an odd number of transpositions.

Let's look at a couple of concrete examples.

Example 4.2.2

For $N = 2$, the sequence $\{1, 2\}$ has two permutations:

$$\begin{aligned} p_1 : \{1,2\} &\to \{1,2\}, \quad s(p_1) = +1 \\ p_2 : \{1,2\} &\to \{2,1\}, \quad s(p_2) = -1. \end{aligned} \tag{4.2.15}$$

Plugging these into Equation (4.2.14) yields the previously-discussed two-fermion state (4.2.12).

Example 4.2.3

For $N = 3$, the sequence $\{1, 2, 3\}$ has $3! = 6$ permutations:

$$\begin{aligned} p_1 : \{1,2,3\} &\to \{1,2,3\}, \quad s(p_1) = +1 \\ p_2 : \{1,2,3\} &\to \{2,1,3\}, \quad s(p_2) = -1 \\ p_3 : \{1,2,3\} &\to \{2,3,1\}, \quad s(p_3) = +1 \\ p_4 : \{1,2,3\} &\to \{3,2,1\}, \quad s(p_4) = -1 \\ p_5 : \{1,2,3\} &\to \{3,1,2\}, \quad s(p_5) = +1 \\ p_6 : \{1,2,3\} &\to \{1,3,2\}, \quad s(p_6) = -1. \end{aligned} \tag{4.2.16}$$

The permutations can be generated by consecutive transpositions of elements. Each time we perform a transposition, the sign of $s(p)$ is reversed. Hence, the three-fermion state is

$$\begin{aligned} |\phi_1, \phi_2, \phi_3\rangle = \frac{1}{\sqrt{6}} \Big(&|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle - |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle \\ &+ |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle - |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle \\ &+ |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle - |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle \Big). \end{aligned} \tag{4.2.17}$$

We now see why Equation (4.2.14) describes the N-fermion state. Let us apply $\hat{P}_{ij}$ to it:

$$\begin{aligned} \hat{P}_{ij}|\phi_1, \ldots, \phi_N\rangle &= \frac{1}{\sqrt{N!}} \sum_p s(p)\, \hat{P}_{ij} \big[\cdots |\phi_{p(i)}\rangle \cdots |\phi_{p(j)}\rangle \cdots \big] \\ &= \frac{1}{\sqrt{N!}} \sum_p s(p) \, \big[\cdots |\phi_{p(j)}\rangle \cdots |\phi_{p(i)}\rangle \cdots \big]. \end{aligned} \tag{4.2.18}$$

Within each term in the above sum, the single-particle states for $p(i)$ and $p(j)$ have exchanged places. The resulting term must be an exact match for another term in the original expression for $|\phi_1, \ldots, \phi_N\rangle$, since the sum runs over all possible permutations, except for one difference: the coefficient $s(p)$ must have an *opposite* sign, since the two permutations are related by an exchange. It follows that $\hat{P}_{ij}|\phi_1, \ldots, \phi_N\rangle = -|\phi_1, \ldots, \phi_N\rangle$ for any choice of $i \neq j$.

Distinguishing particles

When studying the phenomenon of entanglement in the previous chapter, we implicitly assumed that the particles are distinguishable. For example, in the EPR thought experiment, we started with the two-particle state

$$|\psi_{\text{EPR}}\rangle = \frac{1}{\sqrt{2}} \Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle \Big), \tag{4.2.19}$$

which appears to be antisymmetric. Does this mean that we cannot prepare $|\psi_{\text{EPR}}\rangle$ using photons (which are bosons)? More disturbingly, we discussed how measuring $\hat{S}_z$ on particle A, and obtaining the result $+\hbar/2$, causes the two-particle state to collapse into $|+z\rangle|-z\rangle$, which is neither symmetric nor antisymmetric. Is this result invalidated if the particles are identical?

The answer to each question is no. The confusion arises because the particle exchange symmetry has to involve an exchange of *all* the degrees of freedom of each particle, and Equation (4.2.19) only shows the spin degree of freedom.

To unpack the above statement, let us suppose the two particles in the EPR experiment are identical bosons. We have focused on each particle's spin degree of freedom, but they must also have a position degree of freedom—that's how we can have a particle at

Alpha Centauri (A) and another at Betelgeuse (B). If we explicitly account for this position degree of freedom, the single-particle Hilbert space should be

$$\mathscr{H}^{(1)} = \mathscr{H}_{\text{spin}} \otimes \mathscr{H}_{\text{position}}. \tag{4.2.20}$$

For simplicity, let us treat position as a twofold degree of freedom, treating $\mathscr{H}_{\text{position}}$ as a 2D space spanned by the basis $\{|A\rangle, |B\rangle\}$.

Now consider the state we previously denoted by $|+z\rangle|-z\rangle$, which refers to a spin-up particle at A and a spin-down particle at B. In our previous notation, it was implicitly assumed that A refers to the left-hand slot of the tensor product, and B refers to the right-hand slot. If we account for the position degrees of freedom, the state is written as

$$|+z, A;\ -z, B\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle\Big), \tag{4.2.21}$$

where the kets are written in the following order:

$$\Big[(\text{spin 1}) \otimes (\text{position 1})\Big] \otimes \Big[(\text{spin 2}) \otimes (\text{position 2})\Big]. \tag{4.2.22}$$

The exchange operator $\hat{P}_{12}$ swaps the two particles' Hilbert spaces—which includes both the position *and* the spin part. Hence, Equation (4.2.21) is explicitly symmetric:

$$\begin{aligned} \hat{P}_{12}\,|+z, A\,;\,-z, B\rangle &= \frac{1}{\sqrt{2}}\Big(|-z\rangle|B\rangle|+z\rangle|A\rangle + |+z\rangle|A\rangle|-z\rangle|B\rangle\Big) \\ &= |+z, A\,;\,-z, B\rangle. \end{aligned} \tag{4.2.23}$$

Likewise, if there is a spin-down particle at A and a spin-up particle at B, the bosonic two-particle state is

$$|-z, A\,;\,+z, B\rangle = \frac{1}{\sqrt{2}}\Big(|-z\rangle|A\rangle|+z\rangle|B\rangle + |+z\rangle|B\rangle|-z\rangle|A\rangle\Big). \tag{4.2.24}$$

Using Equations (4.2.21) and (4.2.24), we can rewrite the EPR singlet state (4.2.19) as

$$\begin{aligned} |\psi_{\text{EPR}}\rangle &= \frac{1}{\sqrt{2}}\Big(|+z, A\,;\,-z, B\rangle - |-z, A\,;\,+z, B\rangle\Big) \\ &= \frac{1}{2}\Big(\,|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle \\ &\qquad - |-z\rangle|A\rangle|+z\rangle|B\rangle - |+z\rangle|B\rangle|-z\rangle|A\rangle\Big). \end{aligned} \tag{4.2.25}$$

This state looks like a mess, but it turns out that we can clarify it with some careful re-ordering. Instead of the ordering (4.2.22), order by spins and then positions:

$$\Big[(\text{spin 1}) \otimes (\text{spin 2})\Big] \otimes \Big[(\text{position 1}) \otimes (\text{position 2})\Big] \tag{4.2.26}$$

Then Equation (4.2.25) can be rewritten as

$$|\psi_{\text{EPR}}\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big) \otimes \frac{1}{\sqrt{2}}\Big(|A\rangle|B\rangle - |B\rangle|A\rangle\Big). \tag{4.2.27}$$

Evidently, even though the spin degrees of freedom form an antisymmetric combination, as described by Equation (4.2.19), the position degrees of freedom in Equation (4.2.27) also have an antisymmetric form, and this allows the two-particle state to meet the bosonic symmetry condition.

Suppose we perform a measurement on $|\psi_{\text{EPR}}\rangle$, and find that the particle at position A has spin $+z$. As usual, a measurement outcome can be associated with a projection operator. Using the ordering (4.2.22), we can write the relevant projection operator as

$$\hat{\Pi} = \Big(|+z\rangle\langle+z| \otimes |A\rangle\langle A|\Big) \otimes \Big(\hat{I} \otimes \hat{I}\Big) + \Big(\hat{I} \otimes \hat{I}\Big) \otimes \Big(|+z\rangle\langle+z| \otimes |A\rangle\langle A|\Big). \tag{4.2.28}$$

This accounts for the fact that the observed phenomenon—spin $+z$ at position A—may refer to either particle. Applying $\hat{\Pi}$ to the EPR state (4.2.25) yields

$$|\psi'\rangle \;=\; \frac{1}{2}\Big(|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle\Big). \tag{4.2.29}$$

Apart from a change in normalization, this is precisely the fermionic state $|+z, A; -z, B\rangle$ defined in Equation (4.2.21). In our earlier notation, this state was simply written as $|+z\rangle|-z\rangle$. This goes to show that particle exchange symmetry is fully compatible with the concepts of partial measurements, entanglement, etc., discussed in the previous chapter.

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4.3: Second Quantization

In the usual tensor product notation, symmetric and antisymmetric states become quite cumbersome to deal with when the number of particles is large. We will now introduce a formalism called **second quantization**, which greatly simplifies manipulations of such multi-particle states. (The reason for the name "second quantization" will not be apparent until later; it is a bad name, but one we are stuck with for historical reasons.)

We start by defining a convenient way to specify states of multiple identical particles, called the **occupation number representation**. Let us enumerate a set of single-particle states, $\{|1\rangle, |2\rangle, |3\rangle, \cdots\}$ that form a complete orthonormal basis for the single-particle Hilbert space $\mathscr{H}^{(1)}$. Then, we build multi-particle states by specifying how many particles are in state $|1\rangle$, denoted n_1; how many are in state $|2\rangle$, denoted n_2; and so on. Thus,

$$|n_1, n_2, n_3, \ldots\rangle \tag{4.3.1}$$

is *defined* as the appropriate symmetric or antisymmetric multi-particle state, constructed using Equation (4.2.6) if we're dealing with bosons (Section 4.2), or using Equation (4.2.14) if we're dealing with fermions (Section 4.2).

Let us run through a couple of examples:

Example 4.3.1

The two-particle state $|0, 2, 0, 0, \ldots\rangle$has both particles in the single-particle state $|2\rangle$. This is only possible if the particles are bosons, since fermions cannot share the same state. Written out in tensor product form, the symmetric state is

$$|0, 2, 0, 0, \ldots\rangle \equiv |2\rangle|2\rangle. \tag{4.3.2}$$

Example 4.3.2

The three-particle state $|1, 1, 1, 0, 0, \ldots\rangle$has one particle each occupying $|1\rangle$, $|2\rangle$, and $|3\rangle$. If the particles are bosons, this corresponds to the symmetric state

$$\begin{aligned} |1, 1, 1, 0, 0, \ldots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &+ |1\rangle|3\rangle|2\rangle + |2\rangle|1\rangle|3\rangle + |3\rangle|2\rangle|1\rangle\Big). \end{aligned} \tag{4.3.3}$$

And if the particles are fermions, the appropriate antisymmetric state is

$$\begin{aligned} |1, 1, 1, 0, 0, \ldots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &- |1\rangle|3\rangle|2\rangle - |2\rangle|1\rangle|3\rangle - |3\rangle|2\rangle|1\rangle\Big). \end{aligned} \tag{4.3.4}$$

Fock space

There is a subtle point that we have glossed over: what Hilbert space do these state vectors reside in? The state $|0, 2, 0, 0, \ldots\rangle$is a bosonic two-particle state, which is a vector in the two-particle Hilbert space $\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}$. However, $\mathscr{H}^{(2)}$ also contains two-particle states that are not symmetric under exchange, which is not allowed for bosons. Thus, it would be more rigorous for us to narrow the Hilbert space to the space of state vectors that are symmetric under exchange. We denote this reduced space by $\mathscr{H}_S^{(2)}$.

Likewise, $|1, 1, 1, 0, \ldots\rangle$is a three-particle state lying in $\mathscr{H}^{(3)}$. If the particles are bosons, we can narrow the space to $\mathscr{H}_S^{(3)}$. If the particles are fermions, we can narrow it to the space of three-particle states that are antisymmetric under exchange, denoted by $\mathscr{H}_A^{(3)}$. Thus, $|1, 1, 1, 0, \ldots\rangle \in \mathscr{H}_{S/A}^{(3)}$ where the subscript S/A depends on whether we are dealing with symmetric states (S) or antisymmetric states (A).

We can make the occupation number representation more convenient to work with by defining an "extended" Hilbert space, called the **Fock space**, that is the space of bosonic/fermionic states *for arbitrary numbers of particles*. In the formal language of linear algebra, the Fock space can be written as

$$\mathscr{H}_{S/A}^F = \mathscr{H}^{(0)} \oplus \mathscr{H}^{(1)} \oplus \mathscr{H}_{S/A}^{(2)} \oplus \mathscr{H}_{S/A}^{(3)} \oplus \mathscr{H}_{S/A}^{(4)} \oplus \cdots \tag{4.3.5}$$

Here, $\oplus$ represents the **direct sum** operation, which combines vector spaces by directly grouping their basis vectors into a larger basis set; if $\mathscr{H}_1$ has dimension d_1 and $\mathscr{H}_2$ has dimension d_2, then $\mathscr{H}_1 \oplus \mathscr{H}_2$ has dimension $d_1 + d_2$. (By contrast, the space $\mathscr{H}_1 \otimes \mathscr{H}_2$, defined via the tensor product, has dimension $d_1 d_2$.) Once again, the subscript S/A depends on whether we are dealing with bosons (S) or fermions (A).

The upshot is that any multi-particle state that we can write down in the occupation number representation, $|n_1, n_2, n_3, \ldots\rangle$, is guaranteed to lie in the Fock space $\mathscr{H}_{S/A}^F$. Moreover, these states form a complete basis for $\mathscr{H}_{S/A}^F$.

In Equation (4.3.5), the first term of the direct sum is $\mathscr{H}^{(0)}$, the "Hilbert space of 0 particles". This Hilbert space contains only one distinct state vector, denoted by

$$|\varnothing\rangle \equiv |0, 0, 0, 0, \ldots\rangle. \tag{4.3.6}$$

This refers to the **vacuum state**, a quantum state in which there are literally no particles. Note that $|\varnothing\rangle$ is *not* the same thing as a zero vector; it has the standard normalization $\langle\varnothing|\varnothing\rangle = 1$. The concept of a "state of no particles" may seem silly, but we will see that there are very good reasons to include it in the formalism.

Another subtle consequence of introducing the Fock space concept is that it is now legitimate to write down quantum states that lack definite particle numbers. For example,

$$\frac{1}{\sqrt{2}}\Big(|1, 0, 0, 0, 0, \ldots\rangle + |1, 1, 1, 0, 0, \ldots\rangle\Big) \tag{4.3.7}$$

is a valid state vector describing the superposition of a one-particle state and a three-particle state. We will revisit the phenomenon of quantum states with indeterminate particle numbers in Section 4.3, and in the next chapter.

Second quantization for bosons

After this lengthy prelude, we are ready to introduce the formalism of second quantization. Let us concentrate on bosons first.

We define an operator called the **boson creation operator**, denoted by $\hat{a}_\mu^\dagger$ and acting in the following way:

$$\hat{a}_\mu^\dagger |n_1, n_2, \ldots, n_\mu, \ldots\rangle = \sqrt{n_\mu + 1}\ |n_1, n_2, \ldots, n_\mu + 1, \ldots\rangle. \tag{4.3.8}$$

In this definition, there is one particle creation operator for each state in the single-particle basis $\{|\varphi_1\rangle, |\varphi_2\rangle, \ldots\}$. Each creation operator is defined as an operator acting on state vectors in the Fock space $\mathscr{H}_S^F$, and has the effect of incrementing the occupation number of its single-particle state by one. The prefactor of $\sqrt{n_\mu + 1}$ is defined for later convenience.

Applying a creation operator to the vacuum state yields a single-particle state:

$$\begin{aligned} \hat{a}_\mu^\dagger |\varnothing\rangle \ &= \ |0, \ldots, 0, 1, 0, 0, \ldots\rangle. \\ &\qquad\quad \leftarrow \mu \end{aligned} \tag{4.3.9}$$

The creation operator's Hermitian conjugate, $\hat{a}_\mu$, is the **boson annihilation operator**. To characterize it, first take the Hermitian conjugate of Equation (4.3.8):

$$\langle n_1, n_2, \ldots | \hat{a}_\mu = \sqrt{n_\mu + 1}\ \langle n_1, n_2, \ldots, n_\mu + 1, \ldots |. \tag{4.3.10}$$

Right-multiplying by another occupation number state $|n_1', n_2', \ldots\rangle$ results in

$$\begin{aligned} \langle n_1, n_2, \ldots | \hat{a}_\mu | n_1', n_2', \ldots\rangle \ &= \sqrt{n_\mu + 1}\ \langle \ldots, n_\mu + 1, \ldots | \ldots, n_\mu', \ldots\rangle \\ &= \sqrt{n_\mu + 1}\ \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2} \cdots \delta_{n_\mu'}^{n_\mu + 1} \cdots \\ &= \sqrt{n_\mu'}\ \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2} \cdots \delta_{n_\mu'}^{n_\mu + 1} \cdots \end{aligned} \tag{4.3.11}$$

From this, we can deduce that

$$\hat{a}_\mu |n_1', n_2', \ldots, n_\mu', \ldots\rangle = \begin{cases} \sqrt{n_\mu'}\ |n_1', n_2', \ldots, n_\mu' - 1, \ldots\rangle, & \text{if } n_\mu' > 0 \\ 0, & \text{if } n_\mu' = 0. \end{cases} \tag{4.3.12}$$

In other words, the annihilation operator decrements the occupation number of a specific single-particle state by one (hence its name). As a special exception, if the given single-particle state is unoccupied ($n_\mu = 0$), applying $\hat{a}_\mu$ results in a zero vector (note that this is *not* the same thing as the vacuum state $|\varnothing\rangle$).

The boson creation/annihilation operators obey the following commutation relations:

$$[\hat{a}_\mu, \hat{a}_\nu] = [\hat{a}_\mu^\dagger, \hat{a}_\nu^\dagger] = 0, \qquad [\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}. \tag{4.3.13}$$

These can be derived by taking the matrix elements with respect to the occupation number basis. We will go through the derivation of the last commutation relation; the others are left as an exercise (Exercise 4.5.5).

To prove that $[\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}$, first consider the case where the creation/annihilation operators act on the same single-particle state:

$$\begin{aligned}
\langle n_1, n_2, \ldots | \hat{a}_\mu \hat{a}_\mu^\dagger | n_1', n_2' \ldots \rangle &= \sqrt{(n_\mu + 1)(n_\mu' + 1)}\, \langle \ldots, n_\mu + 1, \ldots | \ldots, n_\mu' + 1, \ldots \rangle \\
&= \sqrt{(n_\mu + 1)(n_\mu' + 1)}\, \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2}\ \cdots \delta_{n_\mu'+1}^{n_\mu+1} \cdots \\
&= (n_\mu + 1) \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2}\ \cdots \delta_{n_\mu'}^{n_\mu} \cdots \\
\langle n_1, n_2, \ldots | \hat{a}_\mu^\dagger \hat{a}_\mu | n_1', n_2' \ldots \rangle &= \sqrt{n_\mu n_\mu'}\, \langle \ldots, n_\mu - 1, \ldots | \ldots, n_\mu' - 1, \ldots \rangle \\
&= \sqrt{n_\mu n_\mu'} \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2}\ \cdots \delta_{n_\mu'-1}^{n_\mu-1} \cdots \\
&= n_\mu \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2}\ \cdots \delta_{n_\mu'}^{n_\mu} \cdots
\end{aligned} \tag{4.3.14}$$

In the second equation, we were a bit sloppy in handling the $n_\mu = 0$ and $n_\mu' = 0$ cases, but you can check for yourself that the result on the last line remains correct. Upon taking the difference of the two equations, we get

$$\langle n_1, n_2, \ldots | \left(\hat{a}_\mu \hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger \hat{a}_\mu \right) | n_1', n_2' \ldots \rangle = \delta_{n_1'}^{n_1}\ \delta_{n_2'}^{n_2}\ \cdots \delta_{n_\mu'}^{n_\mu} \cdots = \langle n_1, n_2, \ldots | n_1', n_2' \ldots \rangle. \tag{4.3.15}$$

Since the occupation number states form a basis for $\mathscr{H}_S^F$, we conclude that

$$\hat{a}_\mu \hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger \hat{a}_\mu = \hat{I}\,. \tag{4.3.16}$$

Next, consider the case where $\mu \neq \nu$:

$$\begin{aligned}
\langle n_1, \ldots | \hat{a}_\mu \hat{a}_\nu^\dagger | n_1', \ldots \rangle &= \sqrt{(n_\mu + 1)(n_\nu' + 1)}\, \langle \ldots, n_\mu + 1, \ldots, n_\nu, \ldots | \ldots, n_\mu', \ldots, n_\nu' + 1, \ldots \rangle \\
&= \sqrt{n_\mu' n_\nu}\ \delta_{n_1'}^{n_1}\ \cdots \delta_{n_\mu'}^{n_\mu+1} \cdots \delta_{n_\nu'+1}^{n_\nu} \cdots \\
\langle n_1, \ldots | \hat{a}_\nu^\dagger \hat{a}_\mu | n_1', \ldots \rangle &= \sqrt{n_\mu' n_\nu}\, \langle \ldots, n_\mu, \ldots, n_\nu - 1, \ldots | \ldots, n_\mu' - 1, \ldots, n_\nu' \ldots \rangle \\
&= \sqrt{n_\mu' n_\nu}\ \delta_{n_1'}^{n_1}\ \cdots \delta_{n_\mu'-1}^{n_\mu} \cdots \delta_{n_\nu'}^{n_\nu-1} \cdots \\
&= \sqrt{n_\mu' n_\nu}\ \delta_{n_1'}^{n_1}\ \cdots \delta_{n_\mu'}^{n_\mu+1} \cdots \delta_{n_\nu'+1}^{n_\nu} \cdots
\end{aligned} \tag{4.3.17}$$

Hence,

$$\hat{a}_\mu \hat{a}_\nu^\dagger - \hat{a}_\nu^\dagger \hat{a}_\mu = 0 \quad \text{for} \quad \mu \neq \nu. \tag{4.3.18}$$

Combining these two results gives the desired commutation relation, $[\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}$.

Another useful result which emerges from the first part of this proof is that

$$\langle n_1, n_2, \ldots | \hat{a}_\mu^\dagger \hat{a}_\mu | n_1', n_2' \ldots \rangle = n_\mu \langle n_1, n_2, \ldots | n_1', n_2' \ldots \rangle. \tag{4.3.19}$$

Hence, we can define the Hermitian operator

$$\hat{n}_\mu \equiv \hat{a}_\mu^\dagger \hat{a}_\mu, \tag{4.3.20}$$

whose eigenvalue is the occupation number of single-particle state μ.

If you are familiar with the method of creation/annihilation operators for solving the quantum harmonic oscillator, you will have noticed the striking similarity with the particle creation/annihilation operators for bosons. This is no mere coincidence. We will examine the relationship between harmonic oscillators and bosons in the next chapter.

Second quantization for fermions

For fermions, the multi-particle states are antisymmetric. The fermion creation operator can be defined as follows:

$$\begin{aligned}\hat{c}_\mu^\dagger |n_1, n_2, \ldots, n_\mu, \ldots\rangle &= \begin{cases} (-1)^{n_1+n_2+\cdots+n_{\mu-1}} |n_1, n_2, \ldots, n_{\mu-1}, 1, \ldots\rangle & \text{if } n_\mu = 0 \\ 0 & \text{if } n_\mu = 1. \end{cases} \\ &= (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\ \delta_0^{n_\mu} \left|n_1, n_2, \ldots, n_{\mu-1}, 1, \ldots\right\rangle.\end{aligned} \tag{4.3.21}$$

In other words, if state μ is unoccupied, then $\hat{c}_\mu^\dagger$ increments the occupation number to 1, and multiplies the state by an overall factor of $(-1)^{n_1+n_2+\cdots+n_{\mu-1}}$ (i.e, $+1$ if there is an even number of occupied states preceding μ, and -1 if there is an odd number). The role of this factor will be apparent later. Note that this definition requires the single-particle states to be ordered in some way; otherwise, it would not make sense to speak of the states "preceding" μ. It does not matter which ordering we choose, so long as we make *some* choice, and stick to it consistently.

If μ is occupied, applying $\hat{c}_\mu^\dagger$ gives the zero vector. The occupation numbers are therefore forbidden from being larger than 1, consistent with the Pauli exclusion principle.

The conjugate operator, $\hat{c}_\mu$, is the fermion annihilation operator. To see what it does, take the Hermitian conjugate of the definition of the creation operator:

$$\langle n_1, n_2, \ldots, n_\mu, \ldots | \hat{c}_\mu = (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\ \delta_0^{n_\mu} \left\langle n_1, n_2, \ldots, n_{\mu-1}, 1, \ldots\right|. \tag{4.3.22}$$

Right-multiplying this by $|n'_1, n'_2, \ldots\rangle$ gives

$$\langle n_1, n_2, \ldots, n_\mu, \ldots | \hat{c}_\mu | n'_1, n'_2, \ldots\rangle = (-1)^{n_1+\cdots+n_{\mu-1}}\ \delta_{n'_1}^{n_1} \cdots\ \delta_{n'_{\mu-1}}^{n_{\mu-1}} \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1\right) \delta_{n'_{\mu+1}}^{n_{\mu+1}} \ldots \tag{4.3.23}$$

Hence, we deduce that

$$\begin{aligned}\hat{c}_\mu |n'_1, \ldots, n'_\mu, \ldots\rangle &= \begin{cases} 0 & \text{if } n'_\mu = 0 \\ (-1)^{n'_1+\cdots+n'_{\mu-1}} |n'_1, \ldots, n'_{\mu-1}, 0, \ldots\rangle & \text{if } n'_\mu = 1. \end{cases} \\ &= (-1)^{n'_1+\cdots+n'_{\mu-1}}\ \delta_{n'_\mu}^1 \left|n'_1, \ldots, n'_{\mu-1}, 0, \ldots\right\rangle.\end{aligned} \tag{4.3.24}$$

In other words, if state μ is unoccupied, then applying $\hat{c}_\mu$ gives the zero vector; if state μ is occupied, applying $\hat{c}_\mu$ decrements the occupation number to 0, and multiplies the state by the aforementioned factor of ± 1.

With these definitions, the fermion creation/annihilation operators can be shown to obey the following *anticommutation* relations:

Definition: Anticommutation Relations

$$\left\{\hat{c}_\mu, \hat{c}_\nu\right\} = \left\{\hat{c}_\mu^\dagger, \hat{c}_\nu^\dagger\right\} = 0, \qquad \left\{\hat{c}_\mu, \hat{c}_\nu^\dagger\right\} = \delta_{\mu\nu}. \tag{4.3.25}$$

Here, $\{\cdot, \cdot\}$ denotes an anticommutator, which is defined by

$$\left\{\hat{A}, \hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{4.3.26}$$

Similar to the bosonic commutation relations (4.3.13), the anticommutation relations (4.3.25) can be derived by taking matrix elements with occupation number states. We will only go over the last one, $\left\{\hat{c}_\mu, \hat{c}_\nu^\dagger\right\} = \delta_{\mu\nu}$; the others are left for the reader to verify.

First, consider creation/annihilation operators acting on the same single-particle state μ:

$$\begin{aligned}\left\langle \ldots, n_\mu, \ldots \middle| \hat{c}_\mu \hat{c}_\mu^\dagger \middle| \ldots, n'_\mu, \ldots \right\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}} (-1)^{n'_1+\cdots+n'_{\mu-1}} \, \delta_0^{n_\mu} \delta_{n'_\mu}^0 \\ &\quad \times \left\langle n_1, \ldots, n_{\mu-1}, 1, \ldots \middle| n'_1, \ldots, n'_{\mu-1}, 1, \ldots \right\rangle \\ &= \delta_{n'_\mu}^0 \cdot \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \delta_{n'_\mu}^{n_\mu} \cdots\end{aligned} \tag{4.3.27}$$

By a similar calculation,

$$\left\langle \ldots, n_\mu, \ldots \middle| \hat{c}_\mu^\dagger \hat{c}_\mu \middle| \ldots, n'_\mu, \ldots \right\rangle = \delta_{n'_\mu}^1 \cdot \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \delta_{n'_\mu}^{n_\mu} \cdots \tag{4.3.28}$$

By adding these two equations, and using the fact that $\delta_{n'_\mu}^0 + \delta_{n'_\mu}^1 = 1$, we get

$$\left\langle \ldots, n_\mu, \ldots \middle| \left\{ \hat{c}_\mu, \hat{c}_\mu^\dagger \right\} \middle| \ldots, n'_\mu, \ldots \right\rangle = \left\langle \ldots, n_\mu, \ldots \middle| \ldots, n'_\mu, \ldots \right\rangle \tag{4.3.29}$$

And hence,

$$\left\{ \hat{c}_\mu, \hat{c}_\mu^\dagger \right\} = \hat{I} \, . \tag{4.3.30}$$

Next, we must prove that $\left\{ \hat{c}_\mu, \hat{c}_\nu^\dagger \right\} = 0$ for $\mu \neq \nu$. We will show this for $\mu < \nu$ (the $\mu > \nu$ case follows by Hermitian conjugation). This is, once again, by taking matrix elements:

$$\begin{aligned}\left\langle \ldots, n_\mu, \ldots, n_\nu, \ldots \middle| \hat{c}_\mu \hat{c}_\nu^\dagger \middle| \ldots, n'_\mu, \ldots, n'_\nu, \ldots \right\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}} (-1)^{n'_1+\cdots+n'_{\nu-1}} \, \delta_0^{n_\mu} \delta_{n'_\nu}^0 \\ &\quad \times \left\langle \ldots, 1, \ldots, n_\nu, \ldots \middle| \ldots, n'_\mu, \ldots, 1, \ldots \right\rangle \\ &= (-1)^{n'_\mu+\cdots+n'_{\nu-1}} \, \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1 \right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0 \right) \cdots \\ &= (-1)^{1+n_{\mu+1}+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \left(\delta_{n_\mu}^0 \delta_{n'_\mu}^1 \right) \cdots \left(\delta_{n'_\nu}^0 \delta_{n_\nu}^1 \right) \cdots \\ \left\langle \ldots, n_\mu, \ldots, n_\nu, \ldots \middle| \hat{c}_\nu^\dagger \hat{c}_\mu \middle| \ldots, n'_\mu, \ldots, n'_\nu, \ldots \right\rangle &= (-1)^{n_1+\cdots+n_{\nu-1}} (-1)^{n'_1+\cdots+n'_{\mu-1}} \, \delta_1^{n_\nu} \delta_{n'_\mu}^1 \\ &\quad \times \left\langle \ldots, n_\mu, \ldots, 0, \ldots \middle| \ldots, 0, \ldots, n'_\nu, \ldots \right\rangle \\ &= (-1)^{n_\mu+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1 \right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0 \right) \cdots \\ &= (-1)^{0+n_{\mu+1}+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \, \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1 \right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0 \right) \cdots\end{aligned} \tag{4.3.31}$$

The two equations differ by a factor of -1, so adding them gives zero. Putting everything together, we conclude that $\left\{ c_\mu, c_\nu^\dagger \right\} = \delta_{\mu\nu}$, as stated in (4.3.25).

As you can see, the derivation of the fermionic anticommutation relations is quite hairy, in large part due to the $(-1)^{(\cdots)}$ factors in the definitions of the creation and annihilation operators. But once these relations have been derived, we can deal entirely with the creation and annihilation operators, without worrying about the underlying occupation number representation and its $(-1)^{(\cdots)}$ factors. By the way, if we had chosen to omit the $(-1)^{(\cdots)}$ factors in the definitions, the creation and annihilation operators would still satisfy the *anticommutation* relation $\{\hat{c}_\mu, \hat{c}_\nu^\dagger\} = \delta_{\mu\nu}$, but two creation operators or two annihilation operators would *commute* rather than *anticommute*. During subsequent calculations, the "algebra" of creation and annihilation operators ends up being much harder to deal with.

Second-quantized operators

One of the key benefits of second quantization is that it allows us to express multi-particle quantum operators clearly and succinctly, using the creation and annihilation operators defined in Section 4.3 as "building blocks".

Non-interacting particles

Consider a system of *non-interacting* particles. When there is just one particle ($N = 1$), let the single-particle Hamiltonian be $\hat{H}^{(1)}$, which is a Hermitian operator acting on the single-particle Hilbert space $\mathscr{H}^{(1)}$. For general N, the multi-particle Hamiltonian $\hat{H}$ is a Hermitian operator acting on the Fock space $\mathscr{H}^F$. How is $\hat{H}$ related to $\hat{H}^{(1)}$?

Let us take the bosonic case. Then the multi-particle Hamiltonian should be

$$\hat{H} = \sum_{\mu\nu} \hat{a}^\dagger_\mu H_{\mu\nu} \hat{a}_\nu, \quad \text{where} \quad H_{\mu\nu} = \langle \mu | \hat{H}^{(1)} | \nu \rangle, \tag{4.3.32}$$

where $\hat{a}_\mu$ and $\hat{a}^\dagger_\mu$ are the boson creation and annihilation operators, and $|\mu\rangle$, $|\nu\rangle$ refer to single-particle state vectors drawn from some orthonormal basis for $\mathscr{H}^{(1)}$.

To understand why Equation (4.3.32) is right, consider its matrix elements with respect to various states. First, for the vacuum state $|\varnothing\rangle$,

$$\langle \varnothing | \hat{H} | \varnothing \rangle = 0. \tag{4.3.33}$$

This makes sense. Second, consider the matrix elements between single-particle states:

$$\begin{aligned} \langle n_\mu = 1 | \hat{H} | n_\nu = 1 \rangle &= \langle \varnothing | a_\mu \Big(\sum_{\mu'\nu'} \hat{a}^\dagger_{\mu'} H_{\mu'\nu'} \hat{a}_{\nu'} \Big) a^\dagger_\nu | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \langle \varnothing | a_\mu \hat{a}^\dagger_{\mu'} \hat{a}_{\nu'} a^\dagger_\nu | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \delta^\mu_{\mu'} \delta^\nu_{\nu'} \\ &= H_{\mu\nu}. \end{aligned} \tag{4.3.34}$$

This exactly matches the matrix element defined in Equation (4.3.32).

Finally, consider the case where $\{|\mu\rangle\}$ forms an eigenbasis of $\hat{H}_1$. Then

$$\hat{H}^{(1)} |\mu\rangle = E_\mu |\mu\rangle \quad \Rightarrow \quad H_{\mu\nu} = E_\mu \, \delta_{\mu\nu} \quad \Rightarrow \quad \hat{H} = \sum_\mu E_\mu \, \hat{n}_\mu. \tag{4.3.35}$$

As previously noted, $\hat{n}_\mu = \hat{a}^\dagger_\mu \hat{a}_\mu$ is the number operator, an observable corresponding to the occupation number of single-particle state μ. Thus, the total energy is the sum of the single-particle energies, as expected for a system of non-interacting particles.

We can also think of the Hamiltonian $\hat{H}$ as the generator of time evolution. Equation (4.3.32) describes an infinitesimal time step that consists of a superposition of alternative evolution processes. Each term in the superposition, $\hat{a}^\dagger_\mu H_{\mu\nu} \hat{a}_\nu$, describes a particle being annihilated in state ν, and immediately re-created in state μ, which is equivalent to "transferring" a particle from ν to μ. The quantum amplitude for this process is described by the matrix element $H_{\mu\nu}$. This description of time evolution is applicable not just to single-particle states, but also to multi-particle states containing any number of particles.

Note also that the number of particles does not change during time evolution. Whenever a particle is annihilated in a state ν, it is immediately re-created in some state μ. This implies that the Hamiltonian commutes with the total particle number operator:

$$[\hat{H}, \hat{N}] = 0, \quad \text{where} \quad \hat{N} \equiv \sum_\mu \hat{a}^\dagger_\mu a_\mu. \tag{4.3.36}$$

The formal proof for this is left as an exercise (see Exercise 4.5.6). It follows directly from the creation and annihilation operators' commutation relations (for bosons) or anticommuattion relations (for fermions).

Apart from the total energy, other kinds of observables—the total momentum, total angular momentum, etc.—can be expressed in a similar way. Let $\hat{A}^{(1)}$ be a single-particle observable. For a multi-particle system, the operator corresponding to the "total A" is

$$\hat{A} = \sum_{\mu\nu} \hat{a}^\dagger_\mu A_{\mu\nu} \hat{a}_\nu, \quad \text{where} \quad A_{\mu\nu} = \langle \mu | \hat{A}^{(1)} | \nu \rangle. \tag{4.3.37}$$

For fermions, everything from Equation (4.3.32)–(4.3.37) also holds, but with the a operators replaced by fermionic c operators.

Change of basis

A given set of creation and annihilation operators is defined using a basis of single-particle states $\{|\mu\rangle\}$, but such a choice is obviously not unique. Suppose we have a different single-particle basis $\{|\alpha\rangle\}$, such that

$$|\alpha\rangle = \sum_\mu U_{\alpha\mu} |\mu\rangle, \tag{4.3.38}$$

where $U_{\alpha\mu}$ are the elements of a unitary matrix. Let $\hat{a}^\dagger_\alpha$ and $\hat{a}^\dagger_\mu$ denote the creation operators defined using the two different basis (once again, we will use the notation for bosons, but the equations in this section are valid for fermions too). Writing Equation (4.3.38) in terms of the creation operators,

$$\hat{a}^\dagger_\alpha|\varnothing\rangle = \sum_\mu U_{\alpha\mu}\hat{a}^\dagger_\mu|\varnothing\rangle,$$

We therefore deduce that

$$\hat{a}^\dagger_\alpha = \sum_\mu U_{\alpha\mu}\hat{a}^\dagger_\mu, \quad \hat{a}_\alpha = \sum_\mu U^*_{\alpha\mu}\hat{a}_\mu. \tag{4.3.39}$$

Using the unitarity of $U_{\alpha\mu}$, we can verify that $\hat{a}_\alpha$ and $\hat{a}^\dagger_\alpha$ satisfy bosonic commutation relations if and only if $\hat{a}_\mu$ and $\hat{a}^\dagger_\mu$ do so. For fermions, we put c operators in place of a operators in Equation (4.3.39), and use anticommutation rather than commutation relations.

To illustrate how a basis change affects a second quantized Hamiltonian, consider a system of non-interacting particles whose single-particle Hamiltonian is diagonal in the α basis. The multi-particle Hamiltonian is

$$\hat{H} = \sum_\alpha E_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha, \tag{4.3.40}$$

consistent with Equation (4.3.36). Applying Equation (4.3.39),

$$\hat{H} = \sum_{\mu\nu} \hat{a}^\dagger_\mu \left(\sum_\alpha E_\alpha U_{\alpha\mu} U^*_{\alpha\nu} \right) \hat{a}_\nu \tag{4.3.41}$$

Compare this to single-particle bracket

$$\begin{aligned} H_{\mu\nu} \equiv \langle\mu|\hat{H}^{(1)}|\nu\rangle &= \sum_{\alpha\beta}\langle\alpha|U_{\alpha\mu}\hat{H}^{(1)}U^*_{\beta\nu}|\beta\rangle \\ &= \sum_{\alpha\beta} U_{\alpha\mu}U^*_{\beta\nu}\, E_\beta\, \delta_{\alpha\beta} \\ &= \sum_\alpha E_\alpha\, U_{\alpha\mu}U^*_{\alpha\nu}. \end{aligned} \tag{4.3.42}$$

This precisely matches the term in parentheses in Equation (4.3.41). This is consistent with the general form of $\hat{H}$ for non-interacting particles, Equation (4.3.32).

Particle interactions

Hermitian operators can also be constructed out of other kinds of groupings of creation and annihilation operators. For example, a pairwise (two-particle) potential can be described with a superposition of creation and annihilation operator pairs, of the form

$$\hat{V} = \frac{1}{2}\sum_{\mu\nu\lambda\sigma} \hat{a}^\dagger_\mu \hat{a}^\dagger_\nu\, V_{\mu\nu\lambda\sigma}\, \hat{a}_\sigma \hat{a}_\lambda. \tag{4.3.43}$$

The prefactor of $1/2$ is conventional. In terms of time evolution, $\hat{V}$ "transfers" (annihilates and then re-creates) a *pair* of particles during each infinitesimal time step. Since the number of annihilated particles is always equal to the number of created particles, the interaction conserves the total particle number. We can ensure that $\hat{V}$ is Hermitian by imposing a constraint on the coefficents:

$$\hat{V}^\dagger = \frac{1}{2}\sum_{\mu\nu\lambda\sigma} \hat{a}^\dagger_\lambda \hat{a}^\dagger_\sigma\, V^*_{\mu\nu\lambda\sigma}\, \hat{a}_\nu \hat{a}_\mu = \hat{V} \quad \Leftarrow \quad V^*_{\lambda\sigma\mu\nu} = V_{\mu\nu\lambda\sigma}. \tag{4.3.44}$$

Suppose we are given the two-particle potential as an operator $\hat{V}^{(2)}$ acting on the two-particle Hilbert space $\mathscr{H}^{(2)}$. We should be able to express the second-quantized operator $\hat{V}$ in terms of $\hat{V}^{(2)}$, by comparing their matrix elements. For example, consider the two-boson states

$$\begin{aligned} |n_\mu = 1, n_\nu = 1\rangle &= \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle\Big), \\ |n_\lambda = 1, n_\sigma = 1\rangle &= \frac{1}{\sqrt{2}}\Big(|\lambda\rangle|\sigma\rangle + |\sigma\rangle|\lambda\rangle\Big), \end{aligned} \tag{4.3.45}$$

where $\mu \neq \nu$ and $\lambda \neq \sigma$. The matrix elements of $\hat{V}^{(2)}$ are

$$\begin{aligned} &\langle n_\mu = 1, n_\nu = 1|\hat{V}^{(2)}|n_\lambda = 1, n_\sigma = 1\rangle \\ &= \frac{1}{2}\Big(\langle\mu|\langle\nu|\hat{V}^{(2)}|\lambda\rangle\sigma\rangle + \langle\nu|\langle\mu|\hat{V}^{(2)}|\lambda\rangle\sigma\rangle + \langle\mu|\langle\nu|\hat{V}^{(2)}|\sigma\rangle\lambda\rangle + \langle\nu|\langle\mu|\hat{V}^{(2)}|\sigma\rangle\lambda\rangle\Big). \end{aligned} \tag{4.3.46}$$

On the other hand, the matrix elements of the second-quantized operator $\hat{V}$ are

$$\langle n_\mu = 1, n_\nu = 1|\hat{V}|n_\lambda = 1, n_\sigma = 1\rangle = \sum_{\mu'\nu'\lambda'\sigma'} V_{\mu'\nu'\lambda'\sigma'} \langle\varnothing|\hat{a}_\nu\hat{a}_\mu\hat{a}^\dagger_{\mu'}\hat{a}^\dagger_{\nu'}\hat{a}_{\sigma'}\hat{a}_{\lambda'}\hat{a}^\dagger_\lambda\hat{a}^\dagger_\sigma|\varnothing\rangle \tag{4.3.47}$$

$$= \frac{1}{2}(V_{\mu\nu\lambda\sigma} + V_{\mu\nu\sigma\lambda} + V_{\nu\mu\lambda\sigma} + V_{\nu\mu\sigma\lambda}). \tag{4.3.48}$$

In going from Equation (4.3.47) to (4.3.48), we use the bosonic commutation relations repeatedly to "pushing" the annihilation operators to the right (so that they can act upon $|\varnothing\rangle$) and the creation operators to the left (so that they can act upon $\langle\varnothing|$). Comparing Equation (4.3.46) to Equation (4.3.48), we see that the matrix elements match if we take

$$V_{\mu\nu\lambda\sigma} = \langle\mu|\langle\nu|\hat{V}^{(2)}|\lambda\rangle|\sigma\rangle. \tag{4.3.49}$$

For instance, if the bosons have a position representation, we would have something like

$$V_{\mu\nu\lambda\sigma} = \int d^d r_1 \int d^d r_2 \; \varphi^*_\mu(r_1)\, \varphi^*_\nu(r_2)\, V(r_1, r_2)\, \varphi_\lambda(r_1)\, \varphi_\sigma(r_2). \tag{4.3.50}$$

The appropriate coefficients for $\mu = \nu$ and/or $\lambda = \sigma$, as well as for the fermionic case, are left for the reader to work out.

Other observables?

Another way to build a Hermitian operator from creation and annihilation operators is

$$\hat{A} = \sum_\mu \left(\alpha_\mu \hat{a}^\dagger_\mu + \alpha^*_\mu \hat{a}_\mu\right). \tag{4.3.51}$$

If such a term is added to a Hamiltonian, it breaks the conservation of total particle number. Each infinitesimal time step will include processes that decrement the particle number (due to $\hat{a}_\mu$), as well as processes that increment the particle number (due to $\hat{a}^\dagger_\mu$). Even if the system starts out with a fixed number of particles, such as the vacuum state $|\varnothing\rangle$, it subsequently evolves into a superposition of states with different particle numbers. In the theory of quantum electrodynamics, this type of operator is used to describe the emission and absorption of photons caused by moving charges.

Incidentally, the name "second quantization" comes from this process of using creation and annihilation operators to define Hamiltonians. The idea is that single-particle quantum mechanics is derived by "quantizing" classical Hamiltonians via the imposition of commutation relations like $[x, p] = i\hbar$. Then, we extend the theory to multi-particle systems by using the single-particle states to define creation/annihilation operators obeying commutation or anticommutation relations. This can be viewed as a "second" quantization step.

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4.4: Quantum Field Theory

Field operators

So far, we have been agnostic about the nature of the single-particle states $\{|\varphi_1\rangle, |\varphi_2\rangle, \ldots\}$ used to construct the creation and annihilation operators. Let us now consider the special case where these quantum states are representable by wavefunctions. Let $|\mathbf{r}\rangle$ denote a position eigenstate for a d-dimensional space. A single-particle state $|\varphi_\mu\rangle$ has a wavefunction

$$\varphi_\mu(\mathbf{r}) = \langle \mathbf{r}|\varphi_\mu\rangle. \tag{4.4.1}$$

Due to the completeness and orthonormality of the basis, these wavefunctions satisfy

$$\begin{aligned} \int d^d r\, \varphi_\mu^*(\mathbf{r})\,\varphi_\nu(\mathbf{r}) &= \langle\varphi_\mu| \left(\int d^d r\, |\mathbf{r}\rangle\langle\mathbf{r}|\right) |\varphi_\nu\rangle = \delta_{\mu\nu}, \\ \sum_\mu \varphi_\mu^*(\mathbf{r})\varphi_\mu(\mathbf{r}') &= \langle\mathbf{r}'| \left(\sum_\mu |\varphi_\mu\rangle\langle\varphi_\mu|\right) |\mathbf{r}\rangle = \delta^d(\mathbf{r}-\mathbf{r}'). \end{aligned} \tag{4.4.2}$$

We can use the wavefunctions and the creation/annihilation operators to construct a new and interesting set of operators. For simplicity, suppose the particles are bosons, and let

$$\hat\psi(\mathbf{r}) = \sum_\mu \varphi_\mu(\mathbf{r})\,\hat a_\mu, \qquad \hat\psi^\dagger(\mathbf{r}) = \sum_\mu \varphi_\mu^*(\mathbf{r})\,\hat a_\mu^\dagger. \tag{4.4.3}$$

Using the aforementioned wavefunction properties, we can derive the inverse relations

$$\hat a_\mu = \int d^d r\, \varphi_\mu^*(\mathbf{r})\,\hat\psi(\mathbf{r}), \qquad \hat a_\mu^\dagger = \int d^d r\, \varphi_\mu(\mathbf{r})\,\hat\psi^\dagger(\mathbf{r}). \tag{4.4.4}$$

From the commutation relations for the bosonic a_μ and $a_\mu^\dagger$ operators, we can show that

$$\left[\hat\psi(\mathbf{r}), \hat\psi(\mathbf{r}')\right] = \left[\hat\psi^\dagger(\mathbf{r}), \hat\psi^\dagger(\mathbf{r}')\right] = 0, \quad \left[\hat\psi(\mathbf{r}), \hat\psi^\dagger(\mathbf{r}')\right] = \delta^d(\mathbf{r}-\mathbf{r}'). \tag{4.4.5}$$

In the original commutation relations, the operators for different single-particle states commute; now, the operators for different *positions* commute. A straightforward interpretion for the operators $\hat\psi^\dagger(\mathbf{r})$ and $\hat\psi(\mathbf{r})$ is that they respectively create and annihilate one particle at a point $\mathbf{r}$ (rather than one particle in a given eigenstate).

It is important to note that $\mathbf{r}$ here does not play the role of an observable. It is an *index*, in the sense that each $\mathbf{r}$ is associated with distinct $\hat\psi(\mathbf{r})$ and $\hat\psi^\dagger(\mathbf{r})$ operators. These $\mathbf{r}$-dependent operators serve to generalize the classical concept of a **field**. In a classical field theory, each point $\mathbf{r}$ is assigned a set of numbers corresponding to physical quantities, such as the electric field components $E_x(\mathbf{r})$, $E_y(\mathbf{r})$, and $E_z(\mathbf{r})$. In the present case, each $\mathbf{r}$ is assigned a set of quantum operators. This kind of quantum theory is called a **quantum field theory**.

We can use the $\hat\psi(\mathbf{r})$ and $\hat\psi^\dagger(\mathbf{r})$ operators to write second quantized observables in a way that is independent of the choice of single-particle basis wavefunctions. As discussed in the previous section, given a Hermitian single-particle operator $\hat A_1$ we can define a multi-particle observable $\hat A = \sum_{\mu\nu} \hat a_\mu^\dagger A_{\mu\nu} \hat a_\nu$, where $A_{\mu\nu} = \langle\varphi_\mu|\hat A_1|\varphi_\nu\rangle$. This multi-particle observable can be re-written as

$$\hat A = \int d^d r\, d^d r'\; \hat\psi^\dagger(\mathbf{r})\; \langle\mathbf{r}|\hat A_1|\mathbf{r}'\rangle\; \hat\psi(\mathbf{r}'), \tag{4.4.6}$$

which makes no explicit reference to the single-particle basis states.

For example, consider the familiar single-particle Hamiltonian describing a particle in a potential $V(\mathbf{r})$:

$$\hat H_1 = \hat T_1 + \hat V_1, \quad \hat T_1 = \frac{|\hat{\mathbf{p}}|^2}{2m}, \quad \hat V_1 = V(\hat{\mathbf{r}}), \tag{4.4.7}$$

where $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are position and momentum operators (single-particle observables). The corresponding second quantized operators for the kinetic energy and potential energy are

$$\begin{aligned}\hat{T} &= \frac{\hbar^2}{2m}\int d^d r\; d^d r'\; \hat{\psi}^\dagger(\mathbf{r})\left(\int \frac{d^d k}{(2\pi)^d}\;|\mathbf{k}|^2\; e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\right)\;\hat{\psi}(\mathbf{r}') \\ &= \frac{\hbar^2}{2m}\int d^d r\;\nabla\hat{\psi}^\dagger(\mathbf{r})\cdot\nabla\hat{\psi}(\mathbf{r}) \\ \hat{V} &= \int d^d r\;\hat{\psi}^\dagger(\mathbf{r})\;V(\mathbf{r})\;\hat{\psi}(\mathbf{r}).\end{aligned} \tag{4.4.8}$$

(In going from the first to the second line, we performed integrations by parts.) This result is strongly reminiscent of the expression for the expected kinetic and potential energies in single-particle quantum mechanics:

$$\langle T\rangle = \frac{\hbar^2}{2m}\int d^d r|\nabla\psi(\mathbf{r})|^2, \quad \langle V\rangle = \int d^d r\;V(\mathbf{r})\;|\psi(\mathbf{r})|^2, \tag{4.4.9}$$

where $\psi(\mathbf{r})$ is the single-particle wavefunction.

How are the particle creation and annihilation operators related to the classical notion of "the value of a field at point $\mathbf{r}$", like an electric field $\mathbf{E}(\mathbf{r})$ or magnetic field $\mathbf{B}(\mathbf{r})$? Field variables are measurable quantities, and should be described by Hermitian operators. As we have just seen, Hermitian operators corresponding to the kinetic and potential energy can be constructed via *products* of $\hat{\psi}^\dagger(\mathbf{r})$ with $\hat{\psi}(\mathbf{r})$. But there is another type of Hermitian operator that we can construct by taking *linear combinations* of of $\hat{\psi}^\dagger(\mathbf{r})$ with $\hat{\psi}(\mathbf{r})$. One example is

$$\psi(\mathbf{r}) + \psi(\mathbf{r})^\dagger. \tag{4.4.10}$$

Other possible Hermitian operators have the form

$$F(\mathbf{r}) = \int d^d r'\left(f(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}) + f^*(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}')\right), \tag{4.4.11}$$

where $f(\mathbf{r},\mathbf{r}')$ is some complex function. As we shall see, it is this type of Hermitian operator that corresponds to the classical notion of a field variable like an electric or magnetic field.

In the next two sections, we will try to get a better understanding of the relationship between classical fields and *bosonic* quantum fields. (For fermionic quantum fields, the situation is more complicated; they cannot be related to classical fields of the sort we are familiar with, for reasons that lie outside the scope of this course.)

Revisiting the harmonic oscillator

Before delving into the links between classical fields and bosonic quantum fields, it is first necessary to revisit the harmonic oscillator, to see how the concept of a **mode of oscillation** carries over from classical to quantum mechanics.

A classical harmonic oscillator is described by the Hamiltonian

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{4.4.12}$$

where x is the "position" of the oscillator, which we call the **oscillator variable**; p is the corresponding momentum variable; m is the mass; and ω is the natural frequency of oscillation. We know that the classical equation of motion has the general form

$$x(t) = \mathcal{A}\,e^{-i\omega t} + \mathcal{A}^*\,e^{i\omega t}. \tag{4.4.13}$$

This describes an oscillation of frequency ω. It is parameterized by the **mode amplitude** $\mathcal{A}$, a complex number that determines the magnitude and phase of the oscillation.

For the quantum harmonic oscillator, x and p are replaced by the Hermitian operators $\hat{x}$ and $\hat{p}$. From these, the operators $\hat{a}$ and $\hat{a}^\dagger$ can be defined:

$$\begin{cases}\hat{a} = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\hat{x} + \dfrac{i\hat{p}}{m\omega}\right), \\ \hat{a}^\dagger = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\hat{x} - \dfrac{i\hat{p}}{m\omega}\right).\end{cases} \quad\Leftrightarrow\quad \begin{cases}\hat{x} = \sqrt{\dfrac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \\ \hat{p} = -i\sqrt{\dfrac{m\omega\hbar}{2}}\left(\hat{a} - \hat{a}^\dagger\right).\end{cases} \tag{4.4.14}$$

We can then show that

$$\left[\,\hat{a}\,,\,\hat{a}^{\dagger}\,\right]=1,\quad \hat{H}=\hbar\omega\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right), \tag{4.4.15}$$

and from these the energy spectrum of the quantum harmonic oscillator can be derived. These facts should have been covered in an earlier course.

Here, we are interested in how the creation and annihilation operators relate to the *dynamics* of the quantum harmonic oscillator. In the Heisenberg picture, with $t=0$ as the reference time, we define the time-dependent operator

$$\hat{x}(t)=\hat{U}^{\dagger}(t)\,\hat{x}\,\hat{U}(t),\quad \hat{U}(t)\equiv\exp\!\left(-\frac{i}{\hbar}\hat{H}t\right). \tag{4.4.16}$$

We will adopt the convention that all operators written with an explicit time dependence are Heisenberg picture operators, while operators without an explicit time dependence are Schrödinger picture operators; hence, $\hat{x}\equiv\hat{x}(0)$. The Heisenberg picture creation and annihilation operators, $\hat{a}^{\dagger}(t)$ and $\hat{a}(t)$, are related to $\hat{x}(t)$ by

$$\hat{x}(t)=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}(t)+\hat{a}^{\dagger}(t)\right). \tag{4.4.17}$$

The Heisenberg equation for the annihilation operator is

$$\begin{aligned}\frac{d\hat{a}(t)}{dt}&=\frac{i}{\hbar}\left[\hat{H},\hat{a}(t)\right]\\&=\frac{i}{\hbar}\,\hat{U}^{\dagger}(t)\left[\hat{H},\hat{a}\right]\hat{U}(t)\\&=\frac{i}{\hbar}\,\hat{U}^{\dagger}(t)\Big(-\hbar\omega\hat{a}\Big)\hat{U}(t)\\&=-i\omega\hat{a}(t).\end{aligned} \tag{4.4.18}$$

Hence, the solution for this differential equation is

$$\hat{a}(t)=\hat{a}\,e^{-i\omega t}, \tag{4.4.19}$$

and Equation (4.4.17) becomes

$$\hat{x}(t)=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}\,e^{-i\omega t}+\hat{a}^{\dagger}\,e^{i\omega t}\right). \tag{4.4.20}$$

This has exactly the same form as the classical oscillatory solution (4.4.13)! Comparing the two, we see that $\hat{a}$ times the scale factor $\sqrt{\hbar/2m\omega}$ plays the role of the mode amplitude $\mathcal{A}$.

Now, suppose we come at things from the opposite end. Let's say we start with creation and annihilation operators satisfying Equation (4.4.15), from which Equations (4.4.18)–(4.4.19) follow. Using the creation and annihilation operators, we would like to construct an observable that corresponds to a classical oscillator variable. A natural Hermitian ansatz is

$$\hat{x}(t)=\mathcal{C}\left(\hat{a}\,e^{-i\omega t}+\hat{a}^{\dagger}\,e^{i\omega t}\right), \tag{4.4.21}$$

where $\mathcal{C}$ is a constant that is conventionally taken to be real.

How might $\mathcal{C}$ be chosen? A convenient way is to study the behavior of the oscillator variable *in the classical limit*. The classical limit of a quantum harmonic oscillator is described by a **coherent state**. The details of how this state is defined need not concern us for now (see Appendix E). The most important things to know are that (i) it can be denoted by $|\alpha\rangle$ where $\alpha\in\mathbb{C}$, (ii) it is an eigenstate of the annihilation operator:

$$\hat{a}|\alpha\rangle=\alpha|\alpha\rangle. \tag{4.4.22}$$

And (iii) its energy expectation value is

$$\langle E\rangle=\langle\alpha|\hat{H}|\alpha\rangle=\hbar\omega\left(|\alpha|^2+\frac{1}{2}\right)\overset{|\alpha|^2\to\infty}{\longrightarrow}\hbar\omega|\alpha|^2. \tag{4.4.23}$$

When the system is in a coherent state, we can effectively substitute the $\hat{a}$ and $\hat{a}^\dagger$ operators in Equation (4.4.21) with the complex numbers α and α^*, which gives a classical trajectory

$$x_{\text{classical}}(t) = \mathcal{C}\left(\alpha\, e^{-i\omega t} + \alpha^*\, e^{i\omega t}\right). \tag{4.4.24}$$

This trajectory has amplitude $2\mathcal{C}|\alpha|$. At maximum displacement, the classical momentum is zero, so the total energy of the classical oscillator must be

$$E_{\text{classical}} = \frac{1}{2} m\omega^2 \Big(2\mathcal{C}|\alpha|\Big)^2 = 2m\omega^2\mathcal{C}^2|\alpha|^2. \tag{4.4.25}$$

Equating the classical energy (4.4.25) to the coherent state energy (4.4.23) gives

$$\mathcal{C} = \sqrt{\frac{\hbar}{2m\omega}}, \tag{4.4.26}$$

which is precisely the scale factor found in Equation (4.4.20).

A scalar boson field

We now have the tools available to understand the connection between a very simple classical field and its quantum counterpart. Consider a classical scalar field variable $f(x,t)$, defined in one spatial dimension, whose classical equation of motion is the wave equation:

$$\frac{\partial^2 f(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 f(x,t)}{\partial t^2}. \tag{4.4.27}$$

The constant c is a wave speed. This sort of classical field arises in many physical contexts, including the propagation of sound through air, in which case c is the speed of sound.

For simplicity, let us first assume that the field is defined within a finite interval of length L, with periodic boundary conditions: $f(x,t) \equiv f(x+L,t)$. Solutions to the wave equation can be described by the following ansatz:

$$f(x,t) = \sum_n \left(\mathcal{A}_n\, \varphi_n(x)\, e^{-i\omega_n t} + \mathcal{A}_n^*\, \varphi_n^*(x)\, e^{i\omega_n t}\right). \tag{4.4.28}$$

This ansatz describes a superposition of **normal modes**. Each normal mode (labelled n) varies harmonically in time with a mode frequency ω_n, and varies in space according to a complex mode profile $\varphi_n(x)$; its overall magnitude and phase is specified by the mode amplitude $\mathcal{A}_n$. The mode profiles are normalized according to some fixed convention, e.g.

$$\int_0^L dx\, |\varphi_n(x)|^2 = 1. \tag{4.4.29}$$

Substituting Equation (4.4.28) into Equation (4.4.27), and using the periodic boundary conditions, gives

$$\varphi_n(x) = \frac{1}{\sqrt{L}} \exp(ik_n x), \quad \omega_n = ck_n = \frac{2\pi c n}{L}, \quad n \in \mathbb{Z}. \tag{4.4.30}$$

These mode profiles are orthonormal:

$$\int_0^L dx\, \varphi_m^*(x)\, \varphi_n(x) = \delta_{mn}. \tag{4.4.31}$$

Each normal mode carries energy. By analogy with the classical harmonic oscillator—see Equations (4.4.24)–(4.4.25)—we assume that the energy density (i.e., energy per unit length) is proportional to the square of the field variable. Let it have the form

$$U(x) = 2\rho \sum_n |\mathcal{A}_n|^2\, |\varphi_n(x)|^2, \tag{4.4.32}$$

where ρ is some parameter that has to be derived from the underlying physical context. For example, for acoustic modes, ρ is the mass density of the underlying acoustic medium; in the next chapter, we will see a concrete example involving the energy density of an electromagnetic mode. From Equation (4.4.32), the total energy is

$$E = \int_0^L dx\; U(x) = 2\rho \sum_n |\mathcal{A}_n|^2. \tag{4.4.33}$$

To quantize the classical field, we treat each normal mode as an independent oscillator, with creation and annihilation operators $\hat{a}_n^\dagger$ and $\hat{a}_n$ satisfying

$$\left[\,\hat{a}_m\,,\,\hat{a}_n^\dagger\right] = \delta_{mn}, \quad \left[\,\hat{a}_m\,,\,\hat{a}_n\right] = \left[\,\hat{a}_m^\dagger\,,\,\hat{a}_n^\dagger\right] = 0. \tag{4.4.34}$$

We then take the Hamiltonian to be that of a set of independent harmonic oscillators:

$$\hat{H} = \sum_n \hbar\omega_n \hat{a}_n^\dagger \hat{a}_n + E_0, \tag{4.4.35}$$

where E_0 is the ground-state energy. Just like in the previous section, we can define a Heisenberg-picture annihilation operator, and solving its Heisenberg equation yields

$$\hat{a}_n(t) = \hat{a}_n e^{-i\omega_n t}. \tag{4.4.36}$$

We then define a Schrödinger picture Hermitian operator of the form

$$\hat{f}\,(x) = \sum_n \mathcal{C}_n \Big(\hat{a}_n \varphi_n(x) + \hat{a}_n^\dagger \varphi_n^*(x)\Big), \tag{4.4.37}$$

where $\mathcal{C}_n$ is a real constant (one for each normal mode). The corresponding Heisenberg picture operator is

$$\hat{f}\,(x,t) = \sum_n \mathcal{C}_n \Big(\hat{a}_n \varphi_n(x)\, e^{-i\omega_n t} + \hat{a}_n^\dagger \varphi_n^*(x)\, e^{i\omega_n t}\Big), \tag{4.4.38}$$

which is the quantum version of the classical solution (4.4.28).

To determine the $\mathcal{C}_n$ scale factors, we consider the classical limit. The procedure is a straightforward generalization of the harmonic oscillator case discussed in Section 4.4. We introduce a state $|\alpha\rangle$ that is a coherent state for all the normal modes; i.e., for any given n,

$$\hat{a}_n|\alpha\rangle = \alpha_n|\alpha\rangle \tag{4.4.39}$$

for some $\alpha_n \in \mathbb{C}$. The energy expectation value is

$$\langle E\rangle = \sum_n \hbar\omega_n |\alpha_n|^2. \tag{4.4.40}$$

In the coherent state, the $\hat{a}_n$ and $\hat{a}_n^\dagger$ operators in Equation (4.4.38) can be replaced with α_n and α_n^* respectively. Hence, we identify $\mathcal{C}_n\alpha_n$ as the classical mode amplitude $\mathcal{A}_n$ in Equation (4.4.28). In order for the classical energy (4.4.33) to match the coherent state energy (4.4.40), we need

$$2\rho|\mathcal{A}_n|^2 = 2\rho|\mathcal{C}_n\alpha_n|^2 = \hbar\omega_n|\alpha_n|^2 \quad \Rightarrow \quad \mathcal{C}_n = \sqrt{\frac{\hbar\omega_n}{2\rho}}. \tag{4.4.41}$$

Hence, the appropriate field operator is

$$\hat{f}\,(x,t) = \sum_n \sqrt{\frac{\hbar\omega_n}{2\rho}} \Big(\hat{a}_n \varphi_n(x)\, e^{-i\omega_n t} + \hat{a}_n^\dagger \varphi_n^*(x)\, e^{i\omega_n t}\Big). \tag{4.4.42}$$

Returning to the Schrödinger picture, and using the explicit mode profiles from Equation (4.4.30), we get

$$\hat{f}\,(x) = \sum_n \sqrt{\frac{\hbar\omega_n}{2\rho L}} \Big(\hat{a}_n e^{ik_n x} + \hat{a}_n^\dagger e^{-ik_n x}\Big). \tag{4.4.43}$$

Finally, if we are interested in the infinite-L limit, we can convert the sum over n into an integral. The result is

$$\hat{f}\,(x) = \int dk \sqrt{\frac{\hbar\omega(k)}{4\pi\rho}} \Big(\hat{a}(k)\, e^{ikx} + \hat{a}^\dagger(k)\, e^{-ikx}\Big), \tag{4.4.44}$$

where $\hat{a}(k)$ denotes a rescaled annihilation operator defined by $\hat{a}_n \to \sqrt{2\pi/L}\,\hat{a}(k)$, satisfying

$$\left[\hat{a}(k)\,,\,\hat{a}^\dagger(k')\right] = \delta(k-k'). \tag{4.4.45}$$

Looking ahead

In the next chapter, we will use these ideas to formulate a quantum theory of electromagnetism. This is a bosonic quantum field theory in which the creation and annihilation operators act upon particles called **photons**—the elementary particles of light. Linear combinations of these photon operators can be used to define Hermitian field operators that correspond to the classical electromagnetic field variables. In the classical limit, the quantum field theory reduces to Maxwell's theory of the electromagnetic field.

It is hard to overstate the importance of quantum field theories in physics. At a fundamental level, all elementary particles currently known to humanity can be described using a quantum field theory called the Standard Model. These particles are roughly divided into two categories. The first consists of "force-carrying" particles: photons (which carry the electromagnetic force), gluons (which carry the strong nuclear force), and the W/Z bosons (which carry the weak nuclear force); these particles are excitations of bosonic quantum fields, similar to the one described in the previous section. The second category consists of "particles of matter", such as electrons, quarks, and neutrinos; these are excitations of *fermionic* quantum fields, whose creation and annihilation operators obey anticommutation relations.

As Wilczek (1999) has pointed out, the modern picture of fundamental physics bears a striking resemblance to the old idea of "luminiferous ether": a medium filling all of space and time, whose vibrations are physically-observable light waves. The key difference, as we now understand, is that the ether is not a classical medium, but one obeying the rules of quantum mechanics. (Another difference, which we have not discussed so far, is that modern field theories can be made compatible with relativity.)

It is quite compelling to think of fields, not individual particles, as the fundamental objects in the universe. This point of view "explains", in a sense, why all particles of the same type have the same properties (e.g., why all electrons in the universe have exactly the same mass). The particles themselves are not fundamental; they are excitations of deeper, more fundamental entities—quantum fields!

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4.5: Exercises

Exercises

Exercise 4.5.1

Consider a system of two identical particles. Each single-particle Hilbert space $\mathscr{H}^{(1)}$ is spanned by a basis $\{|\mu_i\}$. The exchange operator is defined on $\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}$ by

$$P\Big(\sum_{ij} \psi_{ij} |\mu_i\rangle |\mu_j\rangle\Big) \equiv \sum_{ij} \psi_{ij} |\mu_j\rangle |\mu_i\rangle. \tag{4.5.1}$$

Prove that $\hat{P}$ is linear, unitary, and Hermitian. Moreover, prove that the operation is basis-independent: i.e., given any other basis $\{\nu_j\}$ that spans $\mathscr{H}^{(1)}$,

$$P\Big(\sum_{ij} \varphi_{ij} |\nu_i\rangle |\nu_j\rangle\Big) = \sum_{ij} \varphi_{ij} |\nu_j\rangle |\nu_i\rangle. \tag{4.5.2}$$

Exercise 4.5.2

Prove that the exchange operator commutes with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left(\nabla_1^2 + \nabla_2^2\right) + \frac{e^2}{4\pi\varepsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|}. \tag{4.5.3}$$

Exercise 4.5.3

An N-boson state can be written as

$$|\phi_1, \phi_2, \ldots, \phi_N\rangle = \mathcal{N} \sum_p \Big(|\phi_{p(1)}\rangle |\phi_{p(2)}\rangle |\phi_{p(3)}\rangle \cdots |\phi_{p(N)}\rangle\Big). \tag{4.5.4}$$

Prove that the normalization constant is

$$\mathcal{N} = \sqrt{\frac{1}{N! \prod_\mu n_\mu!}}, \tag{4.5.5}$$

where n_μ denotes the number of particles occupying the single-particle state μ.

Exercise 4.5.4

$\mathscr{H}_S^{(N)}$ and $\mathscr{H}_A^{(N)}$ denote the Hilbert spaces of N-particle states that are totally symmetric and totally antisymmetric under exchange, respectively. Prove that

$$\begin{aligned} \dim\left(\mathscr{H}_S^{(N)}\right) &= \frac{(d+N-1)!}{N!(d-1)!}, \\ \dim\left(\mathscr{H}_A^{(N)}\right) &= \frac{d!}{N!(d-N)!}. \end{aligned} \tag{4.5.6}$$

Exercise 4.5.5

Prove that for boson creation and annihilation operators, $[\hat{a}_\mu, \hat{a}_\nu] = [\hat{a}_\mu^\dagger, \hat{a}_\nu^\dagger] = 0$.

Exercise 4.5.6

Let $\hat{A}_1$ be an observable (Hermitian operator) for single-particle states. Given a single-particle basis $\{|\varphi_1\rangle, |\varphi_2\rangle, \ldots\}$, define the bosonic multi-particle observable

$$\hat{A} = \sum_{\mu\nu} a_\mu^\dagger \, \langle \varphi_\mu | \hat{A}_1 | \varphi_\nu \rangle \, a_\nu, \tag{4.5.7}$$

where $a_\mu^\dagger$ and a_μ are creation and annihilation operators satisfying the usual bosonic commutation relations, $[a_\mu, a_\nu] = 0$ and $[a_\mu, a_\nu^\dagger] = \delta_{\mu\nu}$. Prove that $\hat{A}$ commutes with the total number operator:

$$\left[\hat{A}, \sum_\mu a_\mu^\dagger a_\mu\right] = 0. \tag{4.5.8}$$

Next, repeat the proof for a fermionic multi-particle observable

$$\hat{A} = \sum_{\mu\nu} c_\mu^\dagger \, \langle \varphi_\mu | \hat{A}_1 | \varphi_\nu \rangle \, c_\nu, \tag{4.5.9}$$

where $c_\mu^\dagger$ and c_μ are creation and annihilation operators satisfying the fermionic anticommutation relations, $\{c_\mu, c_\nu\} = 0$ and $\{c_\mu, c_\nu^\dagger\} = \delta_{\mu\nu}$. In this case, prove that

$$\left[\hat{A}, \sum_\mu c_\mu^\dagger c_\mu\right] = 0. \tag{4.5.10}$$

Further Reading

[1] Bransden & Joachain, §10.1–10.5

[2] Sakurai, §6

[3] J. M. Leinaas and J. Myrheim, *On the Theory of Identical Particles*, Nuovo Cimento B **37**, 1 (1977).

[4] F. Wilczek, *The Persistence of Ether*, Physics Today **52**, 11 (1999).

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CHAPTER OVERVIEW

5: Quantum Electrodynamics

This chapter gives an introduction to **quantum electrodynamics**, the quantum theory of the electromagnetic field and its interactions with electrons and other charged particles. We begin by formulating a quantum Hamiltonian for an electron in a classical electromagnetic field. Then we study how to quantize Maxwell's equations, arriving at a quantum field theory in which the elementary excitations are photons—particles of light. The final step is to formulate a theory in which electrons and photons are treated on the same quantum mechanical footing, as excitations of underlying quantum fields. Along the way, we will see how relativity can be accommodated with quantum theory.

Quantum electrodynamics is an extremely rich and intricate theory, and we will leave out many important topics. Interested readers are referred to are Dyson's 1951 lecture notes on quantum electrodynamics (Dyson 1951), and Zee's textbook *Quantum Field Theory in a Nutshell* (Zee 2010).

5.1: Quantization of the Lorentz Force Law

5.2: Dirac's Theory of the Electron

5.3: Quantizing The Electromagnetic Field

5.4: The Electron-Photon Interaction

5.5: Exercises

Thumbnail: A Feynman diagram showing the radiation of a gluon when an electron and positron are annihilated. (CC BY-SA 3.0; Joel Holdsworth).

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5.1: Quantization of the Lorentz Force Law

Non-relativistic electrons in an electromagnetic field

Consider a non-relativistic charged particle in an electromagnetic field. As we are mainly interested in the physics of electrons interacting with electromagnetic fields, we henceforth take the electric charge of the particle to be $-e$, where $e = 1.602 \times 10^{-19}$ C is the elementary charge. To describe particles with an arbitrary electric charge q, simply perform the substitution $e \to -q$ in the formulas you will subsequently encounter.

We wish to formulate the Hamiltonian governing the quantum dynamics of such a particle, subject to two simplifying assumptions: (i) the particle has charge and mass but is otherwise "featureless" (i.e., we ignore the spin angular momentum and magnetic dipole moment that real electrons possess), and (ii) the electromagnetic field is treated as a classical field, meaning that the electric and magnetic fields are definite quantities rather than operators. (We will see how to go beyond these simplifications later.)

Classically, the electromagnetic field acts on the particle via the Lorentz force law,

$$\mathbf{F}(\mathbf{r},t) = -e\Big(\mathbf{E}(\mathbf{r},t) + \dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r},t)\Big), \tag{5.1.1}$$

where $\mathbf{r}$ and $\dot{\mathbf{r}}$ denote the position and velocity of the particle, t is the time, and $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields. If no other forces are present, Newton's second law yields the equation of motion

$$m\ddot{\mathbf{r}} = -e\Big(\mathbf{E}(\mathbf{r},t) + \dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r},t)\Big), \tag{5.1.2}$$

where m is the particle's mass. To quantize this, we must first convert the equation of motion into the form of Hamilton's equations of motion.

Let us introduce the electromagnetic scalar and vector potentials $\Phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$:

$$\mathbf{E}(\mathbf{r},t) = -\nabla\Phi(\mathbf{r},t) - \frac{\partial \mathbf{A}}{\partial t}, \tag{5.1.3}$$

$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t). \tag{5.1.4}$$

We now postulate that the equation of motion (5.1.2) can be described by the Lagrangian

Definition: Lagrangian

$$L(\mathbf{r},\dot{\mathbf{r}},t) = \frac{1}{2}m\dot{\mathbf{r}}^2 + e\Big[\Phi(\mathbf{r},t) - \dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)\Big]. \tag{5.1.5}$$

This follows the usual prescription for the Lagrangian as kinetic energy minus potential energy, with $-e\Phi$ serving as the potential energy function, except for the $-e\dot{\mathbf{r}}\cdot\mathbf{A}$ term. To see if this Lagrangian works, plug it into the Euler-Lagrange equations

$$\frac{\partial L}{\partial r_i} = \frac{d}{dt}\frac{\partial L}{\partial \dot{r}_i}. \tag{5.1.6}$$

The partial derivatives of the Lagrangian are:

$$\begin{aligned} \frac{\partial L}{\partial r_i} &= e\Big[\partial_i\Phi - \dot{r}_j\,\partial_i A_j\Big] \\ \frac{\partial L}{\partial \dot{r}_i} &= m\dot{r}_i - eA_i. \end{aligned} \tag{5.1.7}$$

Now we want to take the *total* time derivative of $\partial L/\partial\dot{r}_i$. In doing so, note that the $\mathbf{A}$ field has its own t-dependence, as well as varying with the particle's t-dependent position. Thus,

$$\begin{aligned} \frac{d}{dt}\frac{\partial L}{\partial \dot{r}_i} &= m\ddot{r}_i - e\,\frac{d}{dt}A_i(\mathbf{r}(t),t) \\ &= m\ddot{r}_i - e\,\partial_t A_i - e\,\dot{r}_j\partial_j A_i. \end{aligned} \tag{5.1.8}$$

(In the above equations, $\partial_i \equiv \partial/\partial r_i$, where r_i is the i-th component of the position vector, while $\partial_t \equiv \partial/\partial t$.) Plugging these expressions into the Euler-Lagrange equations (5.1.6) gives

$$\begin{aligned} m\ddot{r}_i &= -e\Big[\Big(-\partial_i\Phi - \partial_t A_i\Big) + \dot{r}_j\Big(\partial_i A_j - \partial_j A_i\Big)\Big] \\ &= -e\Big[E_i(\mathbf{r},t) + \big(\dot{\mathbf{r}}\times\mathbf{B}(\mathbf{r},t)\big)_i\Big]. \end{aligned} \tag{5.1.9}$$

(The last step can be derived by expressing the cross product using the Levi-Cevita symbol, and using the identity $\varepsilon_{ijk}\varepsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$.) This exactly matches Equation (5.1.2), as desired.

We now use the Lagrangian to derive the Hamiltonian. The canonical momentum is

$$p_i = \frac{\partial L}{\partial \dot{r}_i} = m\dot{r}_i - eA_i. \tag{5.1.10}$$

The Hamiltonian is defined as $H(\mathbf{r},\mathbf{p}) = \mathbf{p}\cdot\dot{\mathbf{r}} - L$. Using Equation (5.1.10), we express it in terms of $\mathbf{p}$ rather than $\dot{\mathbf{r}}$:

$$\begin{aligned} H &= \mathbf{p}\cdot\left(\frac{\mathbf{p}+e\mathbf{A}}{m}\right) - \left(\frac{|\mathbf{p}+e\mathbf{A}|^2}{2m} + e\Phi - \frac{e}{m}(\mathbf{p}+e\mathbf{A})\cdot\mathbf{A}\right) \\ &= \frac{|\mathbf{p}+e\mathbf{A}|^2}{m} - \frac{e}{m}\mathbf{A}\cdot(\mathbf{p}+e\mathbf{A}) - \left(\frac{|\mathbf{p}+e\mathbf{A}|^2}{2m} + e\Phi - \frac{e}{m}(\mathbf{p}+e\mathbf{A})\cdot\mathbf{A}\right). \end{aligned} \tag{5.1.11}$$

After cancelling various terms, we obtain

$$H = \frac{|\mathbf{p}+e\mathbf{A}(\mathbf{r},t)|^2}{2m} - e\Phi(\mathbf{r},t). \tag{5.1.12}$$

This looks a lot like the Hamiltonian for a non-relativistic particle in a scalar potential,

$$H = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{r},t). \tag{5.1.13}$$

In Equation (5.1.12), the $-e\Phi$ term acts like a potential energy, which is no surprise. More interestingly, the vector potential appears via the substitution

$$\mathbf{p} \to \mathbf{p} + e\mathbf{A}(\mathbf{r},t). \tag{5.1.14}$$

What does this mean? Think about what "momentum" means for a charged particle in an electromagnetic field. Noether's theorem states that each symmetry of a system (whether classical or quantum) is associated with a conservation law. Momentum is the quantity conserved when the system is symmetric under spatial translations. One of Hamilton's equations states that

$$\frac{dp_i}{dt} = \frac{\partial H}{\partial r_i}, \tag{5.1.15}$$

which implies that if H is $\mathbf{r}$-independent, then $d\mathbf{p}/dt = 0$. But when the electromagnetic potentials are $\mathbf{r}$-independent, the quantity $m\dot{\mathbf{r}}$ (which we usually call momentum) is not necessarily conserved! Take the potentials

$$\Phi(\mathbf{r},t) = 0, \quad \mathbf{A}(\mathbf{r},t) = Ct\hat{z}, \tag{5.1.16}$$

where C is some constant. These potentials are $\mathbf{r}$-independent, but the vector potential is time-dependent, so the $-\dot{\mathbf{A}}$ term in Equation (5.1.4) gives a non-vanishing electric field:

$$\mathbf{E}(\mathbf{r},t) = -C\hat{z}, \quad \mathbf{B}(\mathbf{r},t) = 0. \tag{5.1.17}$$

The Lorentz force law then says that

$$\frac{d}{dt}(m\dot{\mathbf{r}}) = eC\hat{z}, \tag{5.1.18}$$

and thus $m\dot{\mathbf{r}}$ is not conserved. On the other hand, the quantity $\mathbf{p} = m\dot{\mathbf{r}} - e\mathbf{A}$ *is* conserved:

$$\frac{d}{dt}(m\dot{\mathbf{r}} - e\mathbf{A}) = eC\hat{z} - eC\hat{z} = 0. \tag{5.1.19}$$

Hence, this is the appropriate canonical momentum for a particle in an electromagnetic field.

We are now ready to go from classical to quantum mechanics. Replace $\mathbf{r}$ with the position operator $\hat{\mathbf{r}}$, and $\mathbf{p}$ with the momentum operator $\hat{\mathbf{p}}$. The resulting quantum Hamiltonian is

Definition: Quantum Hamiltonian

$$\hat{H}(t) = \frac{|\hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}}, t)|^2}{2m} - e\Phi(\hat{\mathbf{r}}, t). \tag{5.1.20}$$

Note

The momentum operator is $\hat{\mathbf{p}} = -i\hbar\nabla$ in the wavefunction representation, as usual.

Gauge symmetry

The Hamiltonian (5.1.20) possesses a subtle property known as **gauge symmetry**. Suppose we modify the scalar and vector potentials via the substitutions

$$\Phi(\mathbf{r}, t) \rightarrow \Phi(\mathbf{r}, t) - \dot{\Lambda}(\mathbf{r}, t) \tag{5.1.21}$$
$$\mathbf{A}(\mathbf{r}, t) \rightarrow \mathbf{A}(\mathbf{r}, t) + \nabla\Lambda(\mathbf{r}, t), \tag{5.1.22}$$

where $\Lambda(\mathbf{r}, t)$ is an arbitrary scalar field called a **gauge field**. This is the **gauge transformation** of classical electromagnetism, which as we know leaves the electric and magnetic fields unchanged. When applied to the Hamiltonian (5.1.20), it generates a new Hamiltonian

$$\hat{H}_\Lambda(t) = \frac{|\hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}}, t) + e\nabla\Lambda(\hat{\mathbf{r}}, t)|^2}{2m} - e\Phi(\hat{\mathbf{r}}, t) + e\dot{\Lambda}(\hat{\mathbf{r}}, t). \tag{5.1.23}$$

Now suppose $\psi(\mathbf{r}, t)$ is a wavefunction obeying the Schrödinger equation for the original Hamiltonian $\hat{H}$:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}(t)\psi(\mathbf{r}, t) = \left[\frac{|\hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}}, t)|^2}{2m} - e\Phi(\hat{\mathbf{r}}, t)\right]\psi(\mathbf{r}, t). \tag{5.1.24}$$

Then it can be shown that the wavefunction $\psi\ \exp(-ie\Lambda/\hbar)$ automatically satisfies the Schrödinger equation for the transformed Hamiltonian $\hat{H}_\Lambda$:

$$i\hbar\frac{\partial}{\partial t}\left[\psi(\mathbf{r}, t)\ \exp\left(-\frac{ie\Lambda(\mathbf{r}, t)}{\hbar}\right)\right] = \hat{H}_\Lambda(t)\left[\psi(\mathbf{r}, t)\ \exp\left(-\frac{ie\Lambda(\mathbf{r}, t)}{\hbar}\right)\right]. \tag{5.1.25}$$

To prove this, observe how time and space derivatives act on the new wavefunction:

$$\begin{aligned}\frac{\partial}{\partial t}\left[\psi\ \exp\left(-\frac{ie\Lambda}{\hbar}\right)\right] &= \left[\frac{\partial\psi}{\partial t} - \frac{ie}{\hbar}\dot{\Lambda}\,\psi\right]\exp\left(\frac{ie\Lambda}{\hbar}\right)\\ \nabla\left[\psi\ \exp\left(-\frac{ie\Lambda}{\hbar}\right)\right] &= \left[\nabla\psi - \frac{ie}{\hbar}\nabla\Lambda\,\psi\right]\exp\left(\frac{ie\Lambda}{\hbar}\right).\end{aligned} \tag{5.1.26}$$

When the extra terms generated by the $\exp(ie\Lambda/\hbar)$ factor are slotted into the Schrödinger equation, they cancel the gauge terms in the scalar and vector potentials. For example,

$$\left(-i\hbar\nabla + e\mathbf{A} + e\nabla\Lambda\right)\left[\psi\ \exp\left(-\frac{ie\Lambda}{\hbar}\right)\right] = \left[\left(-i\hbar\nabla + e\mathbf{A}\right)\psi\right]\ \exp\left(-\frac{ie\Lambda}{\hbar}\right) \tag{5.1.27}$$

If we apply the $(-i\hbar\nabla + e\mathbf{A} + e\nabla\Lambda)$ operator a second time, it has a similar effect but with the quantity in square brackets on the right-hand side of (5.1.27) taking the place of ψ:

$$\left|-i\hbar\nabla + e\mathbf{A} + e\nabla\Lambda\right|^2\left[\psi\ \exp\left(-\frac{ie\Lambda}{\hbar}\right)\right] = \left[|-i\hbar\nabla + e\mathbf{A}|^2\psi\right]\ \exp\left(-\frac{ie\Lambda}{\hbar}\right). \tag{5.1.28}$$

The remainder of the proof for Equation (5.1.25) can be carried out straightforwardly.

The above result can be stated in a simpler form if the electromagnetic fields are static. In this case, the time-independent electromagnetic Hamiltonian is

$$\hat{H} = \frac{|\hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}})|^2}{2m} - e\Phi(\hat{\mathbf{r}}). \tag{5.1.29}$$

Suppose $\hat{H}$ has eigenenergies $\{E_m\}$ and energy eigenfunctions $\{\psi_m(\mathbf{r})\}$. Then the gauge-transformed Hamiltonian

$$\hat{H}_\Lambda = \frac{|\hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}}) + e\nabla\Lambda(\mathbf{r})|^2}{2m} - e\Phi(\hat{\mathbf{r}}) \tag{5.1.30}$$

has the same energy spectrum $\{E_m\}$, with eigenfunctions $\{\, \psi_m(\mathbf{r}) \exp[-ie\Lambda(\mathbf{r})/\hbar] \,\}$.

The Aharonov-Bohm effect

In quantum electrodynamics, it is the electromagnetic scalar and vector potentials that appear directly in the Hamiltonian, not the electric and magnetic fields. This has profound consequences. For example, even if a charged quantum particle resides in a region with zero magnetic field, it can feel the effect of nonzero *vector potentials* produced by magnetic fluxes elsewhere in space, a phenomenon called the **Aharonov-Bohm effect**.

A simple setting for observing the Aharonov-Bohm effect is shown in the figure below. A particle is trapped in a ring-shaped region (an "annulus"), of radius R and width $d \ll R$. Outside the annulus, we set $-e\Phi \to \infty$ so that the wavefunction vanishes; inside the annulus, we set $\Phi = 0$. We ignore the z-dependence of all fields and wavefunctions, so that the problem is two-dimensional. We define polar coordinates (r, ϕ) with the origin at the ring's center.

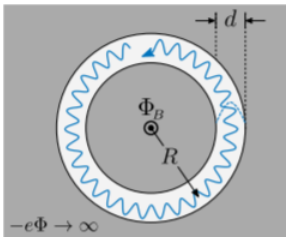

Figure 5.1.1

Now, suppose we thread magnetic flux (e.g., using a solenoid) through the origin, which lies in the region enclosed by the annulus. This flux can be described via the vector potential

$$\mathbf{A}(r, \phi) = \frac{\Phi_B}{2\pi r}\, \mathbf{e}_\phi, \tag{5.1.31}$$

where $\mathbf{e}_\phi$ is the unit vector pointing in the azimuthal direction. We can verify from Equation (5.1.31) that the total magnetic flux through any loop of radius r enclosing the origin is $(\Phi_B/2\pi r)(2\pi r) = \Phi_B$. The fact that this is independent of r implies that the magnetic flux density is concentrated in an infintesimal area surrounding the origin, and zero everywhere else. However, the vector potential $\mathbf{A}$ is nonzero everywhere.

The time-independent Schrödinger equation is

$$\frac{1}{2m}\left| -i\hbar\nabla + \frac{e\Phi_B}{2\pi r}\, \mathbf{e}_\phi \right|^2 \psi(r, \phi) = E\psi(r, \phi), \tag{5.1.32}$$

with the boundary conditions $\psi(R \pm d/2, 0) = 0$. For sufficiently large R, we can guess that the eigenfunctions have the form

$$\psi(r, \phi) \approx \begin{cases} \psi_0 \, \cos\!\left(\frac{\pi}{d}(r - R)\right) e^{ikR\phi}, & r \in [R - d/2, R + d/2] \\ 0 & \text{otherwise.} \end{cases} \tag{5.1.33}$$

This describes a "waveguide mode" with a half-wavelength wave profile in the r direction (so as to vanish at $r = R \pm d/2$), traveling in the azimuthal direction with wavenumber k. The normalization constant ψ_0 is unimportant. We need the wavefunction to be single-valued under a 2π variation in the azimuthal coordinate, so

$$k \cdot 2\pi R = 2\pi n \quad \Rightarrow \quad k = \frac{n}{R}, \quad \text{where} \;\; n \in \mathbb{Z}. \tag{5.1.34}$$

Plugging this into Equation (5.1.32) yields the energy levels

$$E_n = \frac{1}{2m}\left[\left(\frac{n\hbar}{R} + \frac{e\Phi_B}{2\pi R}\right)^2 + \left(\frac{\pi\hbar}{d}\right)^2\right] \tag{5.1.35}$$

$$= \frac{e^2}{8\pi^2 mR^2}\left(\Phi_B + \frac{nh}{e}\right)^2 + \frac{\pi^2\hbar^2}{2md^2}. \tag{5.1.36}$$

These energy levels are sketched versus the magnetic flux Φ_B in the figure below:

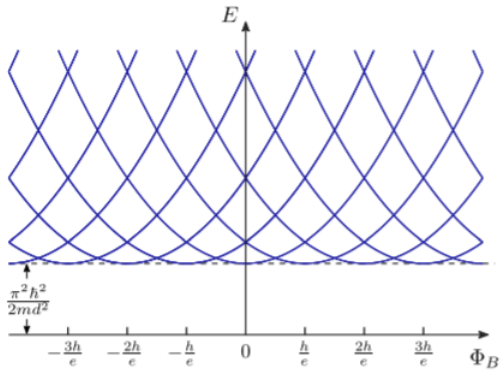

Figure 5.1.2

Each energy level has a quadratic dependence on Φ_B. Variations in Φ_B affect the energy levels despite the fact that $\mathbf{B} = 0$ in the annular region where the electron resides. This is a manifestation of the Aharonov-Bohm effect.

It is noteworthy that the curves of different n are centered at different values of Φ_B corresponding to multiples of $h/e = 4.13567 \times 10^{-5}\ \mathrm{T\,m^2}$, a fundamental unit of magnetic flux called the **magnetic flux quantum**. In other words, changing Φ_B by an exact multiple of h/e leaves the energy spectrum unchanged! This invariance property, which does not depend on the width of the annulus or any other geometrical parameters of the system, can be explained using gauge symmetry. When an extra flux of nh/e (where $n \in \mathbb{Z}$) is threaded through the annulus, Equation (5.1.31) tells us that the change in vector potential is $\boldsymbol{\Delta}\mathbf{A} = (n\hbar/er)\mathbf{e}_\phi$. But we can undo the effects of this via the gauge field

$$\Lambda(r,\phi) = -\frac{n\hbar}{e}\,\phi \quad \Rightarrow \begin{cases} \nabla\Lambda & = (n\hbar/er)\mathbf{e}_\phi \\ e^{-ie\Lambda/\hbar} & = e^{in\phi}. \end{cases} \tag{5.1.37}$$

Note that this Λ is not single-valued, but that's not a problem! Both $\nabla\Lambda$ and the phase factor $\exp(-ie\Lambda/\hbar)$ *are* single-valued, and those are the quantities that enter into the gauge symmetry relations (5.1.21)–(5.1.22).

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5.2: Dirac's Theory of the Electron

The Dirac Hamiltonian

So far, we have been using $p^2/2m$-type Hamiltonians, which are limited to describing non-relativistic particles. In 1928, Paul Dirac formulated a Hamiltonian that can describe electrons moving close to the speed of light, thus successfully combining quantum theory with special relativity. Another triumph of Dirac's theory is that it accurately predicts the magnetic moment of the electron.

Dirac's theory begins from the time-dependent Schrödinger wave equation,

$$i\hbar\,\partial_t\,\psi(\mathbf{r},t) = \hat{H}\psi(\mathbf{r},t). \tag{5.2.1}$$

Note that the left side has a first-order time derivative. On the right, the Hamiltonian $\hat{H}$ contains spatial derivatives in the form of momentum operators. We know that time and space derivatives of wavefunctions are related to energy and momentum by

$$i\hbar\,\partial_t \;\leftrightarrow\; E, \qquad -i\hbar\,\partial_j \;\leftrightarrow\; p_j. \tag{5.2.2}$$

We also know that the energy and momentum of a relativistic particle are related by

$$E^2 = m^2c^4 + \sum_{j=1}^{3} p_j^2 c^2, \tag{5.2.3}$$

where m is the rest mass and c is the speed of light. Note that E and p appear to the same order in this equation. (Following the usual practice in relativity theory, we use Roman indices $j \in \{1,2,3\}$ for the spatial coordinates $\{x,y,z\}$.)

Since the left side of the Schrödinger equation (5.2.1) has a first-order time derivative, a relativistic Hamiltonian should involve first-order spatial derivatives. So we make the guess

$$\hat{H} = \alpha_0 mc^2 + \sum_{j=1}^{3} \alpha_j \hat{p}_j c, \tag{5.2.4}$$

where $\hat{p}_j \equiv -i\hbar\partial/\partial x_j$. The mc^2 and c factors are placed for later convenience. We now need to determine the dimensionless "coefficients" α_0, α_1, α_2, and α_3.

For a wavefunction with definite momentum $\mathbf{p}$ and energy E,

$$\hat{H}\psi = E\psi \quad\Rightarrow\quad \left(\alpha_0 mc^2 + \sum_{j=1}^{3} \alpha_j p_j c\right)\psi = E\,\psi. \tag{5.2.5}$$

This is obtained by replacing the $\hat{p}_j$ operators with definite numbers. If ψ is a scalar, this would imply that $\alpha_0 mc^2 + \sum_j \alpha_j p_j c = E$ for certain scalar coefficients $\{\alpha_0,\ldots,\alpha_3\}$, which does not match the relativistic energy-mass-momentum relation (5.2.3).

But we can get things to work if $\psi(\mathbf{r},t)$ is a multi-component wavefunction, rather than a scalar wavefunction, and the α's are matrices acting on those components via the matrix-vector product operation. In that case,

$$\hat{H} = \hat{\alpha}_0 mc^2 + \sum_{j=1}^{3} \hat{\alpha}_j \hat{p}_j c, \quad \text{where} \;\; \hat{p}_j \equiv -i\hbar\,\partial_j, \tag{5.2.6}$$

where the hats on $\{\hat{\alpha}_0,\ldots,\hat{\alpha}_3\}$ indicate that they are matrix-valued. Applying the Hamiltonian twice gives

$$\left(\hat{\alpha}_0 mc^2 + \sum_{j=1}^{3} \hat{\alpha}_j p_j c\right)^2 \psi = E^2\,\psi. \tag{5.2.7}$$

This can be satisfied if

$$\left(\hat{\alpha}_0 mc^2 + \sum_{j=1}^{3} \hat{\alpha}_j p_j c\right)^2 = E^2\,\hat{I}\,, \tag{5.2.8}$$

where $\hat{I}$ is the identity matrix. Expanding the square (and taking care of the fact that the $\hat{\alpha}_\mu$ matrices need not commute) yields

$$\hat{\alpha}_0^2 m^2 c^4 + \sum_j \left(\hat{\alpha}_0\hat{\alpha}_j + \hat{\alpha}_j\hat{\alpha}_0\right) mc^3 p_j + \sum_{jj'} \hat{\alpha}_j\hat{\alpha}_{j'}\, p_j p_{j'} = E^2\,\hat{I}\,. \tag{5.2.9}$$

This reduces to Equation (5.2.3) if the $\hat{\alpha}_\mu$ matrices satisfy

$$\begin{aligned} \hat{\alpha}_\mu^2 &= \hat{I} \quad \text{for} \;\; \mu = 0,1,2,3, \;\; \text{and} \\ \hat{\alpha}_\mu\hat{\alpha}_\nu + \hat{\alpha}_\nu\hat{\alpha}_\mu &= 0 \quad \text{for} \;\; \mu \neq \nu. \end{aligned} \tag{5.2.10}$$

(We use Greek symbols for indices ranging over the four spacetime coordinates $\{0,1,2,3\}$.) The above can be written more concisely using the anticommutator:

$$\{\hat{\alpha}_\mu, \hat{\alpha}_\nu\} = 2\delta_{\mu\nu}, \quad \text{for} \;\; \mu,\nu = 0,1,2,3. \tag{5.2.11}$$

Also, we need the $\hat{\alpha}_\mu$ matrices to be Hermitian, so that $\hat{H}$ is Hermitian.

It turns out that the smallest possible Hermitian matrices that can satisfy Equation (5.2.11) are 4×4 matrices. The choice of matrices (or "representation") is not uniquely determined. One particularly useful choice is called the **Dirac representation**:

$$\begin{aligned} \hat{\alpha}_0 &= \begin{bmatrix} \hat{I} & \hat{0} \\ \hat{0} & -\hat{I} \end{bmatrix}, \quad \hat{\alpha}_1 = \begin{bmatrix} \hat{0} & \hat{\sigma}_1 \\ \hat{\sigma}_1 & \hat{0} \end{bmatrix} \\ \hat{\alpha}_2 &= \begin{bmatrix} \hat{0} & \hat{\sigma}_2 \\ \hat{\sigma}_2 & \hat{0} \end{bmatrix}, \quad \hat{\alpha}_3 = \begin{bmatrix} \hat{0} & \hat{\sigma}_3 \\ \hat{\sigma}_3 & \hat{0} \end{bmatrix}, \end{aligned} \tag{5.2.12}$$

where $\{\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3\}$ denote the usual Pauli matrices. Since the $\hat{\alpha}_\mu$'s are 4×4 matrices, it follows that $\psi(\mathbf{r})$ is a four-component field.

Eigenstates of the Dirac Hamiltonian

According to Equation (5.2.3), the energy eigenvalues of the Dirac Hamiltonian are

$$E = \pm\sqrt{m^2c^4 + \sum_j p_j^2 c^2}\,. \tag{5.2.13}$$

This is plotted below:

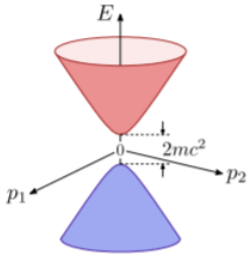

Figure 5.2.2

The energy spectrum forms two hyperbolic bands. For each $\mathbf{p}$, there are two degenerate positive energy eigenvalues, and two degenerate negative energy eigenvalues, for a total of four eigenvalues (matching the number of wavefunction components). The upper band matches the dispersion relation for a massive relativistic particle, as desired. But what about the negative-energy band? Who ordered that?

It might be possible for us to ignore the existence of the negative-energy states, if we only ever consider an isolated electron; we could just declare the positive-energy states to be the ones we are interested in, and ignore the others. However, the problem becomes hard to dismiss once we let the electron interact with another system, such as the electromagnetic field. Under such

circumstances, the availability of negative-energy states extending down to $E \to -\infty$ would destabilize the positive-energy electron states, since the electron can repeatedly hop to states with ever more negative energies by shedding energy (e.g., by emitting photons). This is obviously problematic. However, let us wait for a while (till Section 5.2) to discuss how the stability problem might be resolved.

For now, let us take a closer look at the meaning of the Dirac wavefunction. Its four components represent a four-fold "internal" degree of freedom, distinct from the electron's ordinary kinematic degrees of freedom. Since there are two energy bands, the assignment of an electron to the upper or lower band (or some superposition thereof) consitutes two degrees of freedom. Each band must then posssess a two-fold degree of freedom (so that $2 \times 2 = 4$), which turns out to be associated with the electron's spin.

To see explicitly how this works, let us pick a representation for the $\hat{\alpha}_\mu$ matrices. The choice of representation determines how the four degrees of freedom are encoded in the individual wavefunction components. We will use the Dirac representation (5.2.12). In this case, it is convenient to divide the components into upper and lower parts,

$$\psi(\mathbf{r},t) = \begin{bmatrix} \psi_A(\mathbf{r},t) \\ \psi_B(\mathbf{r},t) \end{bmatrix}, \tag{5.2.14}$$

where ψ_A and ψ_B have two components each. Then, for an eigenstate with energy E and momentum $\mathbf{p}$, applying (5.2.12) to the Dirac equation (5.2.6) gives

$$\psi_A = \frac{1}{E - mc^2} \sum_j \hat{\sigma}_j p_j \psi_B, \tag{5.2.15}$$

$$\psi_B = \frac{1}{E + mc^2} \sum_j \hat{\sigma}_j p_j \psi_A. \tag{5.2.16}$$

Consider the non-relativistic limit, $|\mathbf{p}| \to 0$, for which E approaches either mc^2 or $-mc^2$. For the upper band ($E \gtrsim mc^2$), the vanishing of the denominator in Equation (5.2.15) tells us that the wavefunction is dominated by ψ_A. Conversely, for the lower band ($E \lesssim -mc^2$), Equation (5.2.16) tells us that the wavefunction is dominated by ψ_B. We can thus associate the upper (A) and lower (B) components with the band degree of freedom. Note, however, that this is only an approximate association that holds in the non-relativistic limit! In the relativistic regime, upper-band states can have non-vanishing values in the B components, and vice versa. (There does exist a way to make the upper/lower spinor components correspond rigorously to positive/negative energies, but this requires a more complicated representation than the Dirac representation, for details, see Foldy and Wouthuysen (1950).)

Dirac electrons in an electromagnetic field

To continue pursuing our objective of interpreting the Dirac wavefunction, we must determine how the electron interacts with an electromagnetic field. We introduce electromagnetism by following the same procedure as in the non-relativistic theory (Section 5.1): add $-e\Phi(\mathbf{r},t)$ as a scalar potential function, and add the vector potential via the substitution

$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}},t). \tag{5.2.17}$$

Applying this recipe to the Dirac Hamiltonian (5.2.6) yields

$$i\hbar\,\partial_t \psi = \left\{ \hat{\alpha}_0 mc^2 - e\Phi(\mathbf{r},t) + \sum_j \hat{\alpha}_j \Big[-i\hbar\,\partial_j + eA_j(\mathbf{r},t) \Big] c \right\} \psi(\mathbf{r},t). \tag{5.2.18}$$

You can check that this has the same gauge symmetry properties as the non-relativistic theory discussed in Section 5.1.

In the Dirac representation (5.2.12), Equation (5.2.18) reduces to

$$i\hbar\,\partial_t\,\psi_A \;= \big(+mc^2 - e\Phi\big)\,\psi_A \;+ \sum_j \hat{\sigma}_j \big(-i\hbar\partial_j + eA_j\big)\,c\,\psi_B \tag{5.2.19}$$

$$i\hbar\,\partial_t\,\psi_B \;= \big(-mc^2 - e\Phi\big)\,\psi_B \;+ \sum_j \hat{\sigma}_j \big(-i\hbar\partial_j + eA_j\big)\,c\,\psi_A, \tag{5.2.20}$$

where ψ_A and ψ_B are the previously-introduced two-component objects corresponding to the upper and lower halves of the Dirac wavefunction.

In the non-relativistic limit, solutions to the above equations can be cast in the form

$$\begin{aligned}\psi_A(\mathbf{r},t) &= \Psi_A(\mathbf{r},t)\,\exp\left[-i\left(\frac{mc^2}{\hbar}\right)t\right]\\ \psi_B(\mathbf{r},t) &= \Psi_B(\mathbf{r},t)\,\exp\left[-i\left(\frac{mc^2}{\hbar}\right)t\right].\end{aligned} \tag{5.2.21}$$

The exponentials on the right side are the $\exp(-i\omega t)$ factor corresponding to the rest energy mc^2, which dominates the electron's energy in the non-relativistic limit. (Note that by using $+mc^2$ rather than $-mc^2$, we are explicitly referencing the positive-energy band.) If the electron is in an eigenstate with $\mathbf{p}=0$ and there are no electromagnetic fields, Ψ_A and Ψ_B would just be constants. Now suppose the electron is non-relativistic but not in a $\mathbf{p}=0$ eigenstate, and the electromagnetic fields are weak but not necessarily vanishing. In that case, Ψ_A and Ψ_B are functions that vary with t, but slowly.

Plugging this ansatz into Equations (5.2.19)–(5.2.20) gives

$$i\hbar\,\partial_t\,\Psi_A \;= -e\Phi\;\Psi_A + \sum_j \hat{\sigma}_j\big(-i\hbar\partial_j + eA_j\big)c\;\Psi_B \tag{5.2.22}$$

$$\big(i\hbar\,\partial_t + 2mc^2 + e\Phi\big)\Psi_B \;= \sum_j \hat{\sigma}_j\big(-i\hbar\partial_j + eA_j\big)c\;\Psi_A. \tag{5.2.23}$$

On the left side of Equation (5.2.23), the $2mc^2$ term dominates over the other two, so

$$\Psi_B \;\approx\; \frac{1}{2mc}\sum_j \hat{\sigma}_j\big(-i\hbar\partial_j + eA_j\big)\;\Psi_A. \tag{5.2.24}$$

Plugging this into Equation (5.2.22) yields

$$i\hbar\,\partial_t\,\Psi_A = \left\{-e\Phi \;+\; \frac{1}{2m}\sum_{jk}\hat{\sigma}_j\hat{\sigma}_k\big(-i\hbar\partial_j + eA_j\big)\big(-i\hbar\partial_k + eA_k\big)\right\}\;\Psi_A. \tag{5.2.25}$$

Using the identity $\hat{\sigma}_j\hat{\sigma}_k = \delta_{jk}\hat{I} + i\sum_i \varepsilon_{ijk}\sigma_i$:

$$\begin{aligned}i\hbar\,\partial_t\,\Psi_A \;= \Bigg\{ &-e\Phi \;+\; \frac{1}{2m}\Big|-i\hbar\nabla + e\mathbf{A}\Big|^2\\ &+\; \frac{i}{2m}\sum_{ijk}\varepsilon_{ijk}\hat{\sigma}_i\big(-i\hbar\partial_j + eA_j\big)\big(-i\hbar\partial_k + eA_k\big)\Bigg\}\Psi_A.\end{aligned} \tag{5.2.26}$$

Look carefully at the last term in the curly brackets. Expanding the square yields

$$\frac{i}{2m}\sum_{ijk}\varepsilon_{ijk}\hat{\sigma}_i\Big(-\partial_j\partial_k - i\hbar e\partial_j A_k - i\hbar e\big[A_k\partial_j + A_j\partial_k\big] + e^2A_jA_k\Big). \tag{5.2.27}$$

Due to the antisymmetry of ε_{ijk}, all terms inside the parentheses that are symmetric under j and k cancel out when summed over. The only survivor is the second term, which gives

$$\frac{\hbar e}{2m}\sum_{ijk}\varepsilon_{ijk}\hat{\sigma}_i\partial_j A_k = \frac{\hbar e}{2m}\hat{\boldsymbol{\sigma}}\cdot\mathbf{B}(\mathbf{r},t), \tag{5.2.28}$$

where $\mathbf{B}=\nabla\times\mathbf{A}$ is the magnetic field. Hence,

$$i\hbar\,\partial_t\,\Psi_A = \left\{-e\Phi \;+\; \frac{1}{2m}\Big|-i\hbar\nabla + e\mathbf{A}\Big|^2 \;-\; \left(-\frac{\hbar e}{2m}\,\hat{\boldsymbol{\sigma}}\right)\cdot\mathbf{B}\right\}\Psi_A. \tag{5.2.29}$$

This is an exact match for Equation (5.1.20), except that the Hamiltonian has an additional term of the form $-\hat{\boldsymbol{\mu}}\cdot\hat{\mathbf{B}}$. This additional term corresponds to the potential energy of a magnetic dipole of moment $\boldsymbol{\mu}$ in a magnetic field $\mathbf{B}$. The Dirac theory therefore predicts the electron's magnetic dipole moment to be

$$|\boldsymbol{\mu}| = \frac{\hbar e}{2m}. \tag{5.2.30}$$

Remarkably, this matches the experimentally-observed magnetic dipole moment to about one part in 10^3. The residual mismatch between Equation (5.2.30) and the actual magnetic dipole moment of the electron is understood to arise from quantum fluctuations of the electronic and electromagnetic quantum fields. Using the full theory of quantum electrodynamics, that "anomalous magnetic moment" can also be calculated and matches experiment to around one part in 10^9, making it one of the most precise theoretical predictions in physics! For details, see Zee (2010).

It is noteworthy that we did not set out to include spin in the theory, yet it arose, seemingly unavoidably, as a by-product of formulating a relativistic theory of the electron. This is a manifestation of the general principle that relativistic quantum theory is more constrained than non-relativistic quantum theory Dyson (1951). Due to the demands imposed by relativistic symmetries, spin is not allowed to be an optional part of the theory of the relativistic electron—it has to be built into the theory at a fundamental level.

Positrons and Dirac Field Theory

As noted in Section 5.2, the stability of the quantum states described by the Dirac equation is threatened by the presence of negative-energy solutions. To get around this problem, Dirac suggested that what we regard as the "vacuum" may actually be a state, called the **Dirac sea**, in which all negative-energy states are occupied. Since electrons are fermions, the Pauli exclusion principle would then forbid decay into the negative-energy states, stabilizing the positive-energy states.

At first blush, the idea seems ridiculous; how can the vacuum contain an infinite number of particles? However, we shall see that the idea becomes more plausible if the Dirac equation is reinterpreted as a single-particle *construction* which arises from a more fundamental quantum field theory. The Dirac sea idea is an inherently multi-particle concept, and we know from Chapter 4 that quantum field theory is a natural framework for describing multi-particle quantum states. Let us therefore develop this theory.

Consider again the eigenstates of the single-particle Dirac Hamiltonian with definite momenta and energies. Denote the positive-energy wavefunctions by

$$\frac{u_{\mathbf{k}\sigma}\, e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} = \langle \mathbf{r}|\mathbf{k},+,\sigma\rangle, \quad \text{where } \hat{H}|\mathbf{k},+,\sigma\rangle = \epsilon_{\mathbf{k}\sigma}|\mathbf{k},+,\sigma\rangle. \tag{5.2.31}$$

The negative-energy wavefunctions are

$$\frac{v_{\mathbf{k}\sigma}\, e^{-i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} = \langle \mathbf{r}|\mathbf{k},-,\sigma\rangle, \quad \text{where } \hat{H}|\mathbf{k},-,\sigma\rangle = -\epsilon_{\mathbf{k}\sigma}|\mathbf{k},-,\sigma\rangle. \tag{5.2.32}$$

Note that $|\mathbf{k},-,\sigma\rangle$ denotes a negative-energy eigenstate with momentum $-\hbar\mathbf{k}$, not $\hbar\mathbf{k}$. The reason for this notation, which uses different symbols to label the positive-energy and negative-energy states, will become clear later. Each of the $u_{\mathbf{k}\sigma}$ and $v_{\mathbf{k}\sigma}$ terms are four-component objects (spinors), and for any given $\mathbf{k}$, the set

$$\{u_{\mathbf{k}\sigma}, v_{\mathbf{k},\sigma} \;\mid\; \sigma = 1,2\} \tag{5.2.33}$$

forms an orthonormal basis for the four-dimensional spinor space. Thus,

$$\sum_n \left(u^n_{\mathbf{k}\sigma}\right)^* u^n_{\mathbf{k}\sigma'} = \delta_{\sigma\sigma'}, \quad \sum_n \left(u^n_{\mathbf{k}\sigma}\right)^* v^n_{\mathbf{k}\sigma'} = 0, \quad \text{etc.} \tag{5.2.34}$$

Here we use the notation where $u^n_{\mathbf{k}\sigma}$ is the n-th component of the $u_{\mathbf{k}\sigma}$ spinor, and likewise for the v's.

Following the second quantization procedure from Chapter 4, let us introduce a fermionic Fock space $\mathscr{H}_F$, as well as a set of creation/annihilation operators:

$$\begin{aligned} \hat{b}^\dagger_{\mathbf{k}\sigma} \text{ and } \hat{b}_{\mathbf{k}\sigma} &\text{ create/annihilate } |\mathbf{k},+,\sigma\rangle \\ \hat{d}^\dagger_{\mathbf{k}\sigma} \text{ and } \hat{d}_{\mathbf{k}\sigma} &\text{ create/annihilate } |\mathbf{k},-,\sigma\rangle. \end{aligned} \tag{5.2.35}$$

These obey the fermionic anticommutation relations

$$\begin{aligned} \{\hat{b}_{\mathbf{k}\sigma}, \hat{b}^\dagger_{\mathbf{k}'\sigma'}\} = \delta^3(\mathbf{k}-\mathbf{k}')\,\delta_{\sigma\sigma'}, \quad \{\hat{d}_{\mathbf{k}\sigma}, \hat{d}^\dagger_{\mathbf{k}'\sigma'}\} = \delta^3(\mathbf{k}-\mathbf{k}')\,\delta_{\sigma\sigma'} \\ \{\hat{b}_{\mathbf{k}\sigma}, \hat{b}_{\mathbf{k}'\sigma'}\} = \{\hat{b}_{\mathbf{k}\sigma}, \hat{d}_{\mathbf{k}'\sigma'}\} = \{\hat{d}_{\mathbf{k}\sigma}, \hat{d}_{\mathbf{k}'\sigma'}\} = 0, \quad \text{etc.} \end{aligned} \tag{5.2.36}$$

The Hamiltonian is

$$\hat{H} = \int d^3k \sum_\sigma \epsilon_{\mathbf{k}\sigma} \left(\hat{b}^\dagger_{\mathbf{k}\sigma} \hat{b}_{\mathbf{k}\sigma} - \hat{d}^\dagger_{\mathbf{k}\sigma} \hat{d}_{\mathbf{k}\sigma} \right), \tag{5.2.37}$$

and applying the annihilation operators to the vacuum state $|\varnothing\rangle$ gives zero:

$$\hat{b}_{\mathbf{k}\sigma}|\varnothing\rangle = \hat{d}_{\mathbf{k}\sigma}|\varnothing\rangle = 0. \tag{5.2.38}$$

When formulating bosonic field theory, we defined a local field annihilation operator that annihilates a particle at a given point $\mathbf{r}$. In the infinite-system limit, this took the form

$$\hat{\psi}(\mathbf{r}) = \int d^3k \; \varphi_{\mathbf{k}}(\mathbf{r}) \, \hat{a}_{\mathbf{k}}, \tag{5.2.39}$$

and the orthonormality of the $\varphi_{\mathbf{k}}$ wavefunctions implied that $[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta^3(\mathbf{r}-\mathbf{r}')$. Similarly, we can use the Dirac Hamiltonian's eigenfunctions (5.2.31)–(5.2.32) to define

$$\hat{\psi}_n(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^{3/2}} \sum_\sigma \left(u^n_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \, \hat{b}_{\mathbf{k}\sigma} + v^n_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}} \, \hat{d}_{\mathbf{k}\sigma} \right). \tag{5.2.40}$$

Note that there are two terms in the parentheses because the positive-energy and negative-energy states are denoted by differently-labeled annihilation operators. Moreover, since the wavefunctions are four-component spinors, the field operators have a spinor index n. Using the spinor orthonormality conditions (5.2.34) and the anticommutation relations (5.2.36), we can show that

$$\left\{ \hat{\psi}_n(\mathbf{r}), \hat{\psi}^\dagger_{n'}(\mathbf{r}') \right\} = \delta_{nn'} \, \delta^3(\mathbf{r}-\mathbf{r}'), \tag{5.2.41}$$

with all other anticommutators vanishing. Hence, $\hat{\psi}_n(\mathbf{r})$ can be regarded as an operator that annihilates a four-component fermion at point $\mathbf{r}$.

Now let us *define* the operators

$$\hat{c}_{\mathbf{k}\sigma} = \hat{d}^\dagger_{\mathbf{k}\sigma}. \tag{5.2.42}$$

Using these, the fermionic anticommutation relations can be re-written as

$$\begin{gathered} \{\hat{b}_{\mathbf{k}\sigma}, \hat{b}^\dagger_{\mathbf{k}'\sigma'}\} = \delta^3(\mathbf{k}-\mathbf{k}') \, \delta_{\sigma\sigma'}, \quad \{\hat{c}_{\mathbf{k}\sigma}, \hat{c}^\dagger_{\mathbf{k}'\sigma'}\} = \delta^3(\mathbf{k}-\mathbf{k}') \, \delta_{\sigma\sigma'} \\ \{\hat{b}_{\mathbf{k}\sigma}, \hat{b}_{\mathbf{k}'\sigma'}\} = \{\hat{b}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}\} = \{\hat{c}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}\} = 0, \quad \text{etc.} \end{gathered} \tag{5.2.43}$$

Hence $\hat{c}^\dagger_{\mathbf{k}\sigma}$ and $\hat{c}_{\mathbf{k}\sigma}$ formally satisfy the criteria to be regarded as creation and annihilation operators. The particle created by $\hat{c}^\dagger_{\mathbf{k}\sigma}$ is called a **positron**, and is equivalent to the *absence* of a d-type particle (i.e., a negative-energy electron).

The Hamiltonian (5.2.37) can now be written as

$$\hat{H} = \int d^3k \sum_\sigma \epsilon_{\mathbf{k}\sigma} \left(\hat{b}^\dagger_{\mathbf{k}\sigma} \hat{b}_{\mathbf{k}\sigma} + \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \right) \quad + \quad \text{constant}, \tag{5.2.44}$$

which explicitly shows that the positrons have positive energies (i.e., the absence of a negative-energy particle is equivalent to the presence of a positive-energy particle). With further analysis, which we will skip, it can be shown that the positron created by $\hat{c}^\dagger_{\mathbf{k}\sigma}$ has positive charge e and momentum $\hbar\mathbf{k}$. The latter is thanks to the definition adopted in Equation (5.2.32); the absence of a momentum $-\hbar\mathbf{k}$ particle is equivalent to the presence of a momentum $\hbar\mathbf{k}$ particle. As for the field annihilation operator (5.2.40), it can be written as

$$\hat{\psi}_n(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^{3/2}} \sum_\sigma \left(u^n_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \, \hat{b}_{\mathbf{k}\sigma} + v^n_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}} \, \hat{c}^\dagger_{\mathbf{k}\sigma} \right). \tag{5.2.45}$$

The c-type annihilation operators do *not* annihilate $|\varnothing\rangle$. However, let us define

$$|\varnothing'\rangle = \prod_{\mathbf{k}\sigma} \hat{d}^\dagger_{\mathbf{k}\sigma} |\varnothing\rangle, \tag{5.2.46}$$

which is evidently a formal description of the Dirac sea state. Then

$$\hat{c}_{\mathbf{k}\sigma}|\varnothing'\rangle = \hat{d}^\dagger_{\mathbf{k}\sigma}\prod_{\mathbf{k}'\sigma'}\hat{d}^\dagger_{\mathbf{k}'\sigma'}|\varnothing\rangle = 0. \tag{5.2.47}$$

At the end of the day, we can regard the quantum field theory as being defined in terms of b-type and c-type operators, using the anticommutators (5.2.43), the Hamiltonian (5.2.44), and the field operator (5.2.45), along with the vacuum state $|\varnothing'\rangle$. The elementary particles in this theory are electrons and positrons with strictly positive energies. The single-particle Dirac theory, with its quirky negative-energy states, can then be interpreted as a special construct that maps the quantum field theory into single-particle language. Even though we actually started from the single-particle description, it is the quantum field theory, and its vacuum state $|\varnothing'\rangle$, that is more fundamental.

There are many more details about the Dirac theory that we will not discuss here. One particularly important issue is how the particles transform under Lorentz boosts and other changes in coordinate system. For such details, the reader is referred to Dyson (1951).

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5.3: Quantizing The Electromagnetic Field

Previously (Section 4.4), we have gone through the process of quantizing a scalar boson field. The classical field is decomposed into normal modes, and each mode is quantized by assigning it an independent set of creation and annihilation operators. By comparing the oscillator energies in the classical and quantum regimes, we can derive the Hermitian operator corresponding to the classical field variable, expressed using the creation and annihilation operators. We will use the same approach, with only minor adjustments, to quantize the electromagnetic field.

First, consider a "source-free" electromagnetic field—i.e., with no electric charges and currents. Without sources, Maxwell's equations (in SI units, and in a vacuum) reduce to:

$$\nabla \cdot \mathbf{E} = 0 \tag{5.3.1}$$
$$\nabla \cdot \mathbf{B} = 0 \tag{5.3.2}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{5.3.3}$$
$$\nabla \times \mathbf{B} = \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}. \tag{5.3.4}$$

Once again, we introduce the scalar potential Φ and vector potential $\mathbf{A}$:

$$\mathbf{E} = -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t} \tag{5.3.5}$$
$$\mathbf{B} = \nabla \times \mathbf{A}. \tag{5.3.6}$$

With these relations, Equations (5.3.2) and (5.3.3) are satisfied automatically via vector identities. The two remaining equations, (5.3.1) and (5.3.4), become:

$$\nabla^2\Phi = -\frac{\partial}{\partial t}\nabla \cdot \mathbf{A} \tag{5.3.7}$$
$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = \nabla\left[\frac{1}{c^2}\frac{\partial}{\partial t}\Phi + \nabla \cdot \mathbf{A}\right]. \tag{5.3.8}$$

In the next step, we choose a convenient gauge called the **Coulomb gauge**:

$$\Phi = 0, \quad \nabla \cdot \mathbf{A} = 0. \tag{5.3.9}$$

(To see that we can always make such a gauge choice, suppose we start out with a scalar potential Φ_0 and vector potential $\mathbf{A}_0$ not satisfying (5.3.9). Perform a gauge transformation with a gauge field $\Lambda(\mathbf{r}, t) = -\int^t dt'\ \Phi_0(\mathbf{r}, t')$. The new scalar potential is $\Phi = \Phi_0 + \dot{\Lambda} = 0$; moreover, the new vector potential satisfies

$$\nabla \cdot \mathbf{A} = \nabla \cdot \mathbf{A}_0 - \nabla^2\Lambda = \nabla \cdot \mathbf{A}_0 + \int^t dt'\ \nabla^2\Phi_0(\mathbf{r}, t'). \tag{5.3.10}$$

Upon using Equation (5.3.7), we find that $\nabla \cdot \mathbf{A} = 0$.)

In the Coulomb gauge, Equation (5.3.7) is automatically satisfied. The sole remaining equation, (5.3.8), simplifies to

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A} = 0. \tag{5.3.11}$$

This has plane-wave solutions of the form

$$\mathbf{A}(\mathbf{r}, t) = \left(\mathcal{A}\ e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + \text{c. c.}\right)\mathbf{e}, \tag{5.3.12}$$

where $\mathcal{A}$ is a complex number (the **mode amplitude**) that specifies the magnitude and phase of the plane wave, $\mathbf{e}$ is a real unit vector (the **polarization vector**) that specifies which direction the vector potential points along, and "c.c." denotes the complex conjugate of the first term. Referring to Equation (5.3.11), the angular frequency ω must satisfy

$$\omega = c|\mathbf{k}|. \tag{5.3.13}$$

Moreover, since $\nabla \cdot \mathbf{A} = 0$, it must be the case that

$$\mathbf{k}\cdot\mathbf{e}=0. \tag{5.3.14}$$

In other words, the polarization vector is perpendicular to the propagation direction. For any given $\mathbf{k}$, we can choose (arbitrarily) two orthogonal polarization vectors.

Now suppose we put the electromagnetic field in a box of volume $V=L^3$, with periodic boundary conditions (we will take $L\to\infty$ at the end). The $\mathbf{k}$ vectors form a discrete set:

$$k_j=\frac{2\pi n_j}{L},\quad n_j\in\mathbf{Z},\quad \text{for}\quad j=1,2,3. \tag{5.3.15}$$

Then the vector potential field can be decomposed as a superposition of plane waves,

$$\mathbf{A}(\mathbf{r},t)=\sum_{\mathbf{k}\lambda}\left(\mathcal{A}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}+\text{c. c.}\right)\mathbf{e}_{\mathbf{k}\lambda},\quad \text{where}\quad \omega_{\mathbf{k}}=c|\mathbf{k}|. \tag{5.3.16}$$

Here, λ is a two-fold polarization degree of freedom indexing the two possible orthogonal polarization vectors for each $\mathbf{k}$. (We won't need to specify how exactly these polarization vectors are defined, so long as the definition is used consistently.)

To convert the classical field theory into a quantum field theory, for each $(\mathbf{k},\lambda)$ we define an independent set of creation and annihilation operators:

$$\left[\hat{a}_{\mathbf{k}\lambda},\hat{a}^\dagger_{\mathbf{k}'\lambda'}\right]=\delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'},\quad \left[\hat{a}_{\mathbf{k}\lambda},\hat{a}_{\mathbf{k}'\lambda'}\right]=\left[\hat{a}^\dagger_{\mathbf{k}\lambda},\hat{a}^\dagger_{\mathbf{k}'\lambda'}\right]=0. \tag{5.3.17}$$

Then the Hamiltonian for the electromagnetic field is

$$\hat{H}=\sum_{\mathbf{k}\lambda}\hbar\omega_{\mathbf{k}}\,\hat{a}^\dagger_{\mathbf{k}\lambda}\hat{a}_{\mathbf{k}\lambda},\quad \text{where}\quad \omega_{\mathbf{k}}=c|\mathbf{k}|. \tag{5.3.18}$$

The vector potential is now promoted into a Hermitian operator in the Heisenberg picture:

$$\hat{\mathbf{A}}(\mathbf{r},t)=\sum_{\mathbf{k}\lambda}\mathcal{C}_{\mathbf{k}\lambda}\left(\hat{a}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}+\text{h. c.}\right)\mathbf{e}_{\mathbf{k}\lambda}. \tag{5.3.19}$$

Here, $\mathcal{C}_{\mathbf{k}\lambda}$ is a constant to be determined, and "h.c." denotes the Hermitian conjugate. The creation and annihilation operators in this equation are Schrödinger picture ($t=0$) operators. The particles they create/annihilate are **photons**—elementary particles of light.

To find $\mathcal{C}_{\mathbf{k}\lambda}$, we compare the quantum and classical energies. Suppose the electromagnetic field is in a coherent state $|\alpha\rangle$ such that for any $\mathbf{k}$ and λ,

$$\hat{a}_{\mathbf{k}\lambda}|\alpha\rangle=\alpha_{\mathbf{k}\lambda}|\alpha\rangle \tag{5.3.20}$$

for some $\alpha_{\mathbf{k}\lambda}\in\mathbb{C}$. From this and Equation (5.3.19), we identify the corresponding classical field

$$\mathbf{A}(\mathbf{r},t)=\sum_{\mathbf{k}\lambda}\left(\mathcal{A}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}+\text{c. c.}\right)\mathbf{e}_{\mathbf{k}\lambda},\quad \text{where}\quad \mathcal{C}_{\mathbf{k}\lambda}\alpha_{\mathbf{k}\lambda}=\mathcal{A}_{\mathbf{k}\lambda}. \tag{5.3.21}$$

For each $\mathbf{k}$ and λ, Equations (5.3.5)–(5.3.6) give the electric and magnetic fields

$$\mathbf{E}_{\mathbf{k}\lambda}=\left(i\omega_{\mathbf{k}}\mathcal{A}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}+\text{c. c.}\right)\mathbf{e}_{\mathbf{k}\lambda} \tag{5.3.22}$$

$$\mathbf{B}_{\mathbf{k}\lambda}=\left(i\mathcal{A}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}+\text{c. c.}\right)\mathbf{k}\times\mathbf{e}_{\mathbf{k}\lambda}. \tag{5.3.23}$$

In the classical theory of electromagnetism, Poynting's theorem tells us that the total energy carried by a classical plane electromagnetic wave is

$$\begin{aligned}E&=\int_V d^3r\;\frac{\epsilon_0}{2}\left(|\mathbf{E}_{\mathbf{k}\lambda}|^2+c^2|\mathbf{B}_{\mathbf{k}\lambda}|^2\right)\\&=2\,\epsilon_0\,\omega_{\mathbf{k}}^2\;|\mathcal{A}_{\mathbf{k}\lambda}|^2\,V.\end{aligned} \tag{5.3.24}$$

Here, V is the volume of the enclosing box, and we have used the fact that terms like $e^{2i\mathbf{k}\cdot\mathbf{r}}$ vanish when integrated over $\mathbf{r}$. Hence, we make the correspondence

$$2\,\epsilon_0\,\omega_{\mathbf{k}}^2\,|\mathcal{C}_{\mathbf{k}\lambda}\alpha_{\mathbf{k}\lambda}|^2\,V = \hbar\omega_{\mathbf{k}}|\alpha_{\mathbf{k}\lambda}|^2 \quad \Rightarrow \quad \mathcal{C}_{\mathbf{k}\lambda} = \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}}. \tag{5.3.25}$$

We thus arrive at the result

$$\begin{aligned} \hat{H} &= \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}}\,\hat{a}^\dagger_{\mathbf{k}\lambda}\hat{a}_{\mathbf{k}\lambda} \\ \hat{\mathbf{A}}(\mathbf{r},t) &= \sum_{\mathbf{k}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}}\left(\hat{a}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + \text{h. c.}\right)\mathbf{e}_{\mathbf{k}\lambda} \\ \omega_{\mathbf{k}} &= c|\mathbf{k}|, \quad \left[\hat{a}_{\mathbf{k}\lambda}, \hat{a}^\dagger_{\mathbf{k}'\lambda'}\right] = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}, \quad \left[\hat{a}_{\mathbf{k}\lambda}, \hat{a}_{\mathbf{k}'\lambda'}\right] = 0. \end{aligned} \tag{5.3.26}$$

To describe infinite free space rather than a finite-volume box, we take the $L\to\infty$ limit and re-normalize the creation and annihilation operators by the replacement

$$\hat{a}_{\mathbf{k}\lambda} \to \sqrt{\frac{(2\pi)^3}{V}}\;\hat{a}_{\mathbf{k}\lambda}. \tag{5.3.27}$$

Then the sums over $\mathbf{k}$ become integrals over the infinite three-dimensional space:

$$\begin{aligned} \hat{H} &= \int d^3k \sum_{\lambda} \hbar\omega_{\mathbf{k}}\,\hat{a}^\dagger_{\mathbf{k}\lambda}\hat{a}_{\mathbf{k}\lambda} \\ \hat{\mathbf{A}}(\mathbf{r},t) &= \int d^3k \sum_{\lambda} \sqrt{\frac{\hbar}{16\pi^3\epsilon_0\omega_{\mathbf{k}}}}\left(\hat{a}_{\mathbf{k}\lambda}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + \text{h. c.}\right)\mathbf{e}_{\mathbf{k}\lambda} \\ \omega_{\mathbf{k}} &= c|\mathbf{k}|, \quad \left[\hat{a}_{\mathbf{k}\lambda}, \hat{a}^\dagger_{\mathbf{k}'\lambda'}\right] = \delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}, \quad \left[\hat{a}_{\mathbf{k}\lambda}, \hat{a}_{\mathbf{k}'\lambda'}\right] = 0. \end{aligned} \tag{5.3.28}$$

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5.4: The Electron-Photon Interaction

Having derived quantum theories for the electron and the electromagnetic field, we can put them together to describe how electrons interact with the electromagnetic field by absorbing and/or emitting photons. Here, we present the simplest such calculation.

Let $\mathscr{H}_\text{e}$ be the Hilbert space for one electron, and $\mathscr{H}_\text{EM}$ be the Hilbert space for the electromagnetic field. The combined system is thus described by $\mathscr{H}_e \otimes \mathscr{H}_\text{EM}$. We seek a Hamiltonian of the form

$$H = H_e + H_\text{EM} + H_\text{int}, \tag{5.4.1}$$

where H_e is the Hamiltonian for the "bare" electron, H_EM is the Hamiltonian for the source-free electromagnetic field, and H_int is an **interaction Hamiltonian** describing how the electron interacts with photons.

Let us once again adopt the Coulomb gauge, so that the scalar potential is zero, and the electromagnetic field is solely described via the vector potential. In Section 5.1, we saw that the effect of the vector potential on a charged particle can be described via the substitution

$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}}, t). \tag{5.4.2}$$

In Section 5.2, we saw that this substitution is applicable not just to non-relativistic particles, but also to fully relativistic particles described by the Dirac Hamiltonian. Previously, we have treated the $\mathbf{A}$ in this substitution as a classical object lacking quantum dynamics of its own. Now, we replace it by the vector potential *operator* derived in Section 5.3:

$$\hat{\mathbf{A}}(\hat{\mathbf{r}}, t) = \begin{cases} \displaystyle\sum_{\mathbf{k}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_\mathbf{k} V}} \left(\hat{a}_{\mathbf{k}\lambda}\, e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_\mathbf{k} t)} + \text{h. c.} \right) \mathbf{e}_{\mathbf{k}\lambda}, & \text{(finite volume)} \\ \displaystyle\int d^3k \sum_\lambda \sqrt{\frac{\hbar}{16\pi^3 \epsilon_0 \omega_\mathbf{k}}} \left(\hat{a}_{\mathbf{k}\lambda}\, e^{i(\mathbf{k}\cdot\hat{\mathbf{r}} - \omega_\mathbf{k} t)} + \text{h. c.} \right) \mathbf{e}_{\mathbf{k}\lambda}, & \text{(infinite space).} \end{cases} \tag{5.4.3}$$

Using this, together with either the electronic and electromagnetic Hamiltonians, we can finally describe the photon emission process. Suppose a non-relativistic electron is orbiting an atomic nucleus in an excited state $|1\rangle \in \mathscr{H}_e$. Initially, the photon field is in its vacuum state $|\varnothing\rangle \in \mathscr{H}_\text{EM}$. Hence, the initial state of the combined system is

$$|\psi_i\rangle = |1\rangle \otimes |\varnothing\rangle. \tag{5.4.4}$$

Let H_int be the Hamiltonian term responsible for photon absorption/emission. If $H_\text{int} = 0$, then $|\psi_i\rangle$ would be an energy eigenstate. The atom would remain in its excited state forever.

In actuality, H_int is not zero, so $|\psi_i\rangle$ is not an energy eigenstate. As the system evolves, the excited electron may decay into its ground state $|0\rangle$ by emitting a photon with energy E, equal to the energy difference between the atom's excited state $|1\rangle$ and ground state $|0\rangle$. For a non-relativistic electron, the Hamiltonian (5.1.20) yields the interaction Hamiltonian

$$H_\text{int} = \frac{e}{2m} \left(\hat{\mathbf{p}} \cdot \hat{\mathbf{A}} + \text{h. c.} \right), \tag{5.4.5}$$

where $\hat{\mathbf{A}}$ must now be treated as a field operator, not a classical field.

Consider the states that $|\psi_i\rangle$ can decay into. There is a continuum of possible final states, each having the form

$$|\psi_f^{(\mathbf{k}\lambda)}\rangle = |0\rangle \otimes \left(\hat{a}^\dagger_{\mathbf{k}\lambda} |\varnothing\rangle \right), \tag{5.4.6}$$

which describes the electron being in its ground state and the electromagnetic field containing one photon, with wave-vector $\mathbf{k}$ and polarization λ.

According to Fermi's Golden Rule (see Chapter 2), the decay rate is

$$\kappa = \frac{2\pi}{\hbar} \overline{\left| \langle \psi_f^{(\mathbf{k}\lambda)} | \hat{H}_\text{int} | \psi_i \rangle \right|^2}\, \mathcal{D}(E), \tag{5.4.7}$$

where $\overline{(\cdots)}$ denotes the average over the possible decay states of energy E (i.e., equal to the energy of the initial state), and $\mathcal{D}(E)$ is the density of states.

To calculate the matrix element $\langle\psi_f^{(\mathbf{k}\lambda)}|\hat{H}_{\rm int}|\psi_i\rangle$, let us use the infinite-volume version of the vector field operator (5.4.3). (You can check that using the finite-volume version yields the same results; see Exercise 5.5.2.) We will use the Schrödinger picture operator, equivalent to setting $t=0$ in Equation (5.4.3). Then

$$\begin{aligned}\langle\psi_f^{(\mathbf{k}\lambda)}|\hat{H}_{\rm int}|\psi_i\rangle = \frac{e}{2m}\int d^3k' \sum_{j\lambda}\sqrt{\frac{\hbar}{16\pi^3\epsilon_0\omega_{\mathbf{k}'}}} \\ \times\left(\langle 0|\hat{p}_j e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}|1\rangle + \left\langle 0|e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}\hat{p}_j|1\right\rangle\right) e^j_{\mathbf{k}'\lambda'}\ \langle\varnothing|\hat{a}_{\mathbf{k}\lambda}\hat{a}^\dagger_{\mathbf{k}'\lambda'}|\varnothing\rangle.\end{aligned} \tag{5.4.8}$$

We can now use the fact that $\langle\varnothing|\hat{a}_{\mathbf{k}\lambda}\hat{a}^\dagger_{\mathbf{k}'\lambda'}|\varnothing\rangle = \delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}$. Moreover, we approximate the $\exp(-i\mathbf{k}\cdot\hat{\mathbf{r}})$ factors in the brakets with 1; this is a good approximation since the size of a typical atomic orbital ($\lesssim 10^{-9}$ m) is much smaller than the optical wavelength ($\sim 10^{-6}$ m), meaning that $\exp(-i\mathbf{k}\cdot\mathbf{r})$ does not vary appreciably over the range of positions $\mathbf{r}$ where the orbital wavefunctions are significant. The above equation then simplifies to

$$\langle\psi_f^{(\mathbf{k}\lambda)}|\hat{H}_{\rm int}|\psi_i\rangle \approx \frac{e}{m}\sum_j\sqrt{\frac{\hbar}{16\pi^3\epsilon_0\omega_{\mathbf{k}}}}\ \langle 0|\hat{p}_j|1\rangle\ e^j_{\mathbf{k}\lambda}. \tag{5.4.9}$$

We can make a further simplification by observing that for $\hat{H}_e = |\hat{\mathbf{p}}|^2/2m + V(\mathbf{r})$,

$$[\hat{H}_e,\ \hat{\mathbf{r}}] = -i\hbar\mathbf{p}/m \quad\Rightarrow\quad \langle 0|\hat{p}_j|1\rangle = -\frac{imE\mathbf{d}}{\hbar}. \tag{5.4.10}$$

The complex number $\mathbf{d} = \langle 0|\mathbf{r}|1\rangle$, called the **transition dipole moment**, is easily calculated from the orbital wavefunctions. Thus,

$$\langle\psi_f^{(\mathbf{k}\lambda)}|\hat{H}_{\rm int}|\psi_i\rangle \approx -ie\sqrt{\frac{E}{16\pi^3\epsilon_0}}\ \mathbf{d}\cdot\mathbf{e}_{\mathbf{k}\lambda}. \tag{5.4.11}$$

$$\left|\langle\psi_f^{(\mathbf{k}\lambda)}|\hat{H}_{\rm int}|\psi_i\rangle\right|^2 \approx \frac{e^2E}{16\pi^3\epsilon_0}\ \left|\mathbf{d}\cdot\mathbf{e}_{\mathbf{k}\lambda}\right|^2. \tag{5.4.12}$$

(Check for yourself that Equation (5.4.12) should, and does, have units of $[E^2V]$.) We now need the average over the possible photon states $(\mathbf{k},\lambda)$. In taking this average, the polarization vector runs over all possible directions, and a standard angular integration shows that

$$\overline{\left|\mathbf{d}\cdot\mathbf{e}_{\mathbf{k}\lambda}\right|^2} = \sum_{j=1}^3 |d_j|^2\ \overline{e_j^2} = \sum_{j=1}^3 |d_j|^2\cdot\frac{1}{3} = \frac{|\mathbf{d}|^2}{3}. \tag{5.4.13}$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}, \tag{5.4.14}$$

and defining $\omega = E/\hbar$ as the frequency of the emitted photon. The resulting decay rate is

Definition: Decay Rate

$$\kappa = \frac{4\alpha\omega^3\ \overline{|\mathbf{d}|^2}}{3c^2}. \tag{5.4.15}$$

The figure below compares this prediction to experimentally-determined decay rates for the simplest excited states of hydrogen, lithium, and sodium atoms. The experimental data are derived from atomic emission line-widths, and correspond to the rate of spontaneous emission (also called the "Einstein A coefficient") as the excited state decays to the ground state. For the Fermi's Golden Rule curve, we simply approximated the transition dipole moment as $|\mathbf{d}| \approx 10^{-10}$ m (based on the fact that $|\mathbf{d}|$ has units of length, and the length scale of an atomic orbital is about an angstrom); to be more precise, $\mathbf{d}$ ought to be calculated using the actual orbital wavefunctions. Even with the crude approximations we have made, the predictions are within striking distance of the experimental values.

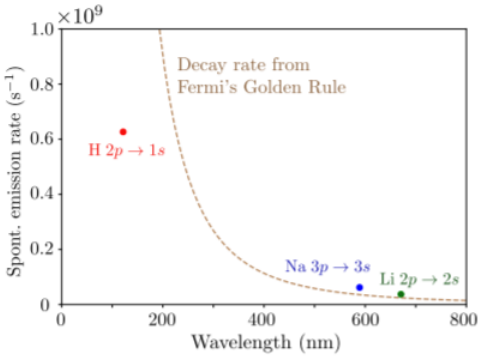

Figure 5.4.1: Spontaneous emission rates (Einstein A coefficients) for the $2p \to 1s$ transition in hydrogen, the $2p \to 2s$ transition in lithium, and the $3p \to 3s$ transition in sodium. Data points extracted from the NIST Atomic Spectra Database (https://www.nist.gov/pml/atomic-spectra-database). The dashed curve shows the decay rate based on Fermi's Golden Rule, with $|\mathbf{d}| \approx 10^{-10}\,\mathrm{m}$.

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5.5: Exercises

Exercises

Exercise 5.5.1

In Section 5.3, we derived the vector potential operator, in an infinite volume, to be

$$\hat{\mathbf{A}}(\mathbf{r},t) = \int d^3k \sum_\lambda \sqrt{\frac{\hbar}{16\pi^3\epsilon_0\omega_\mathbf{k}}} \left(\hat{a}_{\mathbf{k}\lambda}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_\mathbf{k}t)} + \text{h. c.}\right) \mathbf{e}_{\mathbf{k}\lambda}. \tag{5.5.1}$$

Since $[\hat{a}_{\mathbf{k}\lambda}, \hat{a}^\dagger_{\mathbf{k}'\lambda'}] = \delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}$, the creation and annihilation operators each have units of $[x^{3/2}]$. Prove that $\hat{\mathbf{A}}$ has the same units as the classical vector potential.

Exercise 5.5.2

Repeat the spontaneous decay rate calculation from Section 5.4 using the finite-volume versions of the creation/annihilation operators and the vector potential operator (5.4.3). Show that it yields the same result (5.4.16).

Exercise 5.5.3

The density of photon states at energy E is defined as

$$\mathcal{D}(E) = 2\int d^3k\; \delta(E - E_\mathbf{k}), \tag{5.5.2}$$

where $E_\mathbf{k} = \hbar c|\mathbf{k}|$. Note the factor of 2 accounting for the polarizations. Prove that

$$\mathcal{D}(E) = \frac{8\pi E^2}{\hbar^3 c^3}, \tag{5.5.3}$$

and show that $\mathcal{D}(E)$ has units of $[E^{-1}V^{-1}]$.

Further Reading

[1] F. J. Dyson, *1951 Lectures on Advanced Quantum Mechanics Second Edition*, arxiv:quant-ph/0608140.

[2] A. Zee, *Quantum Field Theory in a Nutshell* (Princeton University Press, 2010). [cite:zee]

[3] L. L. Foldy and S. A. Wouthuysen, *On the Dirac Theory of Spin* $1/2$ *Particles and Its Non-Relativistic Limit*, Physical Review **78**, 29 (1950).

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CHAPTER OVERVIEW

6: Appendices

Topic hierarchy

6.1: A- Partial Wave Analysis
6.2: B- The Transfer Matrix Method
6.3: C- Entropy
6.4: D- Numerical Tensor Products
6.5: E- Coherent States

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6.1: A- Partial Wave Analysis

This Appendix describes the method of **partial wave analysis**, which can be used to solve 3D scattering problems with *spherically symmetric* scattering potentials. Such a potential, $V(r)$, depends only on the radial distance $r = \sqrt{x^2+y^2+z^2}$ and not on direction. This typically describes a situation where a point particle or spherically-symmetric object sits at the coordinate origin, $\mathbf{r} = 0$, and is bombarded by incident particles.

A.1 Spherical Waves

We begin by considering "exterior" solutions to the Schrödinger wave equation. Far from the scatterer, where $V(r) \to 0$, the Schrödinger wave equation can be rearranged into

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = 0, \quad \text{where} \quad k = \sqrt{2mE/\hbar^2}. \tag{6.1.1}$$

This partial differential equation is called the **Helmholtz equation**. We emphasize that E plays the role of a tunable parameter, and is not an eigenvalue in an eigenproblem. For the moment, we will not specify the boundary conditions, and look instead for a general set of solutions for a given E (and hence k).

In spherical coordinates (r, θ, ϕ), the Helmholtz equation has the explicit form

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + k^2\psi(r,\theta,\phi) = 0. \tag{6.1.2}$$

There is a standard procedure for solving this. The first step is to perform a separation of variables, and look for solutions of the form

$$\psi(r,\theta,\phi) = A(r)Y_{\ell m}(\theta,\phi), \tag{6.1.3}$$

where $A(r)$ is a function to be determined and $Y_{\ell m}(\theta,\phi)$ is a special function known as a spherical harmonic. Spherical harmonics are functions designed specifically to represent the angular dependence of solutions with definite angular momenta. In the context of quantum mechanics, ℓ and m are the quantum numbers representing the total angular momentum and the z-component of the angular momentum. It can be shown that the indices ℓ and m must be integers satisfying $\ell \geq 0$ and $-\ell \leq m \leq \ell$, in order for $Y_{\ell m}(\theta,\phi)$ to be periodic in ϕ and regular at the poles of the spherical coordinate system.

After plugging in this form for $\psi(r,\theta,\phi)$, the Helmholtz equation reduces to the following ordinary differential equation, which is a variant of the Bessel equation:

$$\frac{d}{dr}\left(r^2\frac{dA}{dr}\right) + \left[k^2r^2 - \ell(\ell+1)\right]A(r) = 0, \quad \ell \in \mathbb{Z}_0^+. \tag{6.1.4}$$

Note that m drops out of the equation. Thus, $A(r)$ depends on ℓ, but *not* on m.

The ordinary differential equation has two linearly independent real solutions, $j_\ell(kr)$ and $y_\ell(kr)$, which are called **spherical Bessel functions**. Most scientific computing packages provide functions to calculate these; Scientific Python, for example, has `scipy.special.spherical_jn` and `scipy.special.spherical_yn`. Some spherical Bessel functions are plotted below:

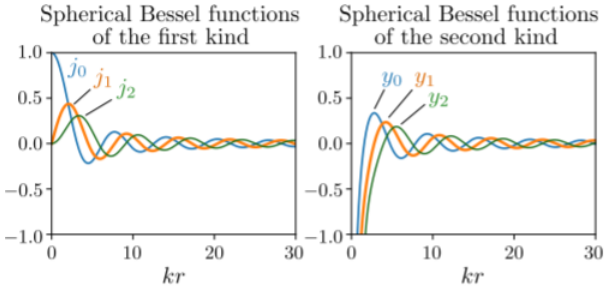

Figure 6.1.1

Note that the y_ℓ functions diverge at $kr \to 0$. This does not bother us, for we are interested in solutions defined in the exterior region, away from the coordinate origin.

For large values of the input, the spherical Bessel functions have the limiting forms

$$\begin{aligned} j_\ell(kr) &\overset{kr\to\infty}{\longrightarrow} \frac{\sin(kr-\frac{\ell\pi}{2})}{kr} \\ y_\ell(kr) &\overset{kr\to\infty}{\longrightarrow} -\frac{\cos(kr-\frac{\ell\pi}{2})}{kr}. \end{aligned} \tag{6.1.5}$$

Since we are interested in incoming and outgoing spherical waves, it is convenient to define

$$h_\ell^\pm(kr) = j_\ell(kr) \pm i y_\ell(kr). \tag{6.1.6}$$

This complex function is called a **spherical Hankel function** of the first kind $(+)$ or second kind $(-)$. It solves the same differential equation, but has the limiting form

$$h_\ell^\pm(kr) \overset{kr\to\infty}{\longrightarrow} \pm\frac{\exp\left[\pm i(kr-\frac{\ell\pi}{2})\right]}{ikr}. \tag{6.1.7}$$

Using it, we can write down a solution to the Helmholtz equation, in the form

$$\Psi_{\ell m}^\pm(\mathbf{r}) = h_\ell^\pm(kr)\, Y_{\ell m}(\theta,\phi). \tag{6.1.8}$$

This describes a spherical wave that is outgoing $(+)$ or incoming $(-)$, and that has a definite angular momentum described by the quantum numbers ℓ and m.

Because the Helmholtz equation is linear, any linear combination of spherical waves, with various values of (ℓ, m), is also a solution:

$$\psi(\mathbf{r}) = \sum_\pm \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell c_{\ell m}^\pm \Psi_{\ell m}^\pm(\mathbf{r}). \tag{6.1.9}$$

It can be shown that the spherical waves form a complete solution basis. In other words, any solution to the 3D Helmholtz equation within the exterior region can be written in the above form, for some choice of complex coefficients $c_{\ell m}^\pm$. (By the way, these spherical waves are appropriately normalized so that the flux associated with each term is directly proportional to $|c_{\ell m}^\pm|^2$.)

A.2 The Scattering Matrix

For a given scattering problem, the exterior wavefunction is described by the complex numbers $\{c_{\ell m}^+\}$ and $\{c_{\ell m}^-\}$. These two sets of coefficients cannot, however, be independent of each other. For fixed $V(\mathbf{r})$ and E, suppose there is an incoming spherical wave with definite angular momentum, say $c_{\ell m}^- = 1$ for some choice of (ℓ, m). After striking the scatterer, the quantum particle bounces back out to infinity, and the outgoing wavefunction is some superposition of outgoing spherical waves with a variety of angular momenta, described by certain coefficients $\{c_{\ell' m'}^+\}$.

Thus, for each choice of incoming wave with definite angular momentum, there is a corresponding set of outgoing-wave coefficients. Since the Schrödinger wave equation is linear, the principle of superposition states that linear combinations of scattering solutions are also valid solutions—i.e., solutions to the Schrödinger wave equation for the same $V(\mathbf{r})$ and E. So if we supply an *arbitrary* set of incoming coefficients $\{c_{\ell m}^-\}$, the outgoing coefficients must be determined by a linear relation of the form

$$c_{\ell m}^+ = \sum_{\ell' m'} S_{\ell m, \ell' m'}\; c_{\ell' m'}^-. \tag{6.1.10}$$

To make the notation cleaner, we rewrite this as

$$c_\mu^+ = \sum_\nu S_{\mu\nu}\, c_\nu^-, \tag{6.1.11}$$

where each μ or ν denotes a pair of angular momentum quantum numbers (ℓ, m), called a **scattering channel**. The matrix S is called a **scattering matrix**. Knowing $V(\mathbf{r})$ and E, we can calculate S, and knowing S we can determine the outgoing wavefunction produced by any set of incoming waves.

Thus far, we have not specified how the "incoming" and "outgoing" waves are related to the "incident" and "scattered" waves of a scattering experiment. We now consider an incident plane wave, $\psi_i(\mathbf{r}) = \Psi_i \exp(i\mathbf{k}_i \cdot \mathbf{r})$, where $|\mathbf{k}_i| = k$. This introduces an important complication: relative to the coordinate origin, a plane wave is neither purely "incoming" nor "outgoing"! In fact, there is a mathematical identity stating that

$$\begin{aligned} e^{i\mathbf{k}_i\cdot\mathbf{r}} &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 4\pi j_\ell(kr) e^{i\ell\pi/2}\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}) \\ &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 2\pi \left[h^+_\ell(kr) + h^-_\ell(kr)\right] e^{i\ell\pi/2}\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}). \end{aligned} \tag{6.1.12}$$

Here, $\hat{\mathbf{k}}_i$ denotes the angular components (in spherical coordinates) of the incident wave-vector $\mathbf{k}_i$, while $\hat{\mathbf{r}}$ likewise denotes the angular components of the position vector $\mathbf{r}$. Equation (6.1.12) informs us that the incident plane wave can be decomposed into a superposition of incoming and outgoing spherical waves, with the wave coefficients

$$c^{\pm}_{i,\ell m} = 2\pi e^{i\ell\pi/2}\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\ \Psi_i. \tag{6.1.13}$$

As described in Chapter 1, the total wavefunction in a scattering problem is the sum of the incident wavefunction $\psi_i(\mathbf{r})$ and the scattered wavefunction $\psi_s(\mathbf{r})$. The latter must be a superposition of only outgoing spherical waves; let us denote the coefficients by $c^+_{s,\ell m}$. The scattering matrix relation can then be re-written as

$$c^+_\mu = c^+_{i,\mu} + c^+_{s,\mu} = \sum_{\mu\nu} S_{\mu\nu} c^-_{i,\nu} \tag{6.1.14}$$

$$\Rightarrow \quad c^+_{s,\ell m} = 2\pi \sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'} \Big) e^{i\ell'\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\ \Psi_i. \tag{6.1.15}$$

Using this, the scattered wavefunction can be written as

$$\begin{aligned} \psi_s(\mathbf{r}) &= \sum_{\ell m} c^+_{s,\ell m} h^+_\ell(kr)\, Y_{\ell m}(\hat{\mathbf{r}}) \\ &= \Psi_i \sum_{\ell m}\sum_{\ell' m'} 2\pi \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'} \Big) e^{i\ell'\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\ h^+_\ell(kr)\, Y_{\ell m}(\hat{\mathbf{r}}). \end{aligned} \tag{6.1.16}$$

Taking the large-r expansion of the spherical Hankel functions yields

$$\psi_s(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} \Psi_i \frac{e^{ikr}}{r} \left[\frac{2\pi}{ik} \sum_{\ell m}\sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'} \Big)\, e^{-i(\ell-\ell')\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\ Y_{\ell m}(\hat{\mathbf{r}}) \right]. \tag{6.1.17}$$

The quantity in square brackets is precisely what we call the scattering amplitude:

$$f(\mathbf{k}_i \to k\hat{\mathbf{r}}) = \frac{2\pi}{ik} \sum_{\ell m}\sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'} \Big)\, e^{-i(\ell-\ell')\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\ Y_{\ell m}(\hat{\mathbf{r}}). \tag{6.1.18}$$

A.3 Spherically Symmetric Scattering Potentials

Generally, the scattering matrix needs to be calculated numerically. The process is greatly simplified if the scattering potential is spherically symmetric, i.e. $V(\mathbf{r}) = V(r)$. In that case, angular momentum is conserved, so an incoming spherical wave with angular momentum quantum numbers (ℓ, m) must scatter exclusively into an outgoing spherical wave with the same (ℓ, m). This means that the scattering matrix components have the form

$$S_{\ell m,\ell' m'} = s_{\ell m}\, \delta_{\ell\ell'}\, \delta_{mm'}. \tag{6.1.19}$$

The scattering amplitude then simplifies to

$$f(\mathbf{k}_i \to k\hat{\mathbf{r}}) = \frac{2\pi}{ik} \sum_{\ell m} \Big(s_{\ell m} - 1 \Big)\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\ Y_{\ell m}(\hat{\mathbf{r}}). \tag{6.1.20}$$

Our task is now to obtain the $s_{\ell m}$'s. The procedure is very similar to what we already went through in Section A.1. The total wavefunction satisfies the Schrödinger wave equation, which can be written in spherical coordinates as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+K^2(r)\psi(r,\theta,\phi)=0, \tag{6.1.21}$$

where

$$K^2(r)=\sqrt{\frac{2m\left[E-V(r)\right]}{\hbar^2}}. \tag{6.1.22}$$

This is similar to the Helmholtz equation, but with the constant k^2 replaced by a function $K^2(r)$. In scattering channel (ℓ,m), the solution has the form

$$\psi(r,\theta,\phi)=A(r)\,Y_{\ell m}(\theta,\phi). \tag{6.1.23}$$

Upon substitution into the Schrödinger wave equation, we find that $A(r)$ must satisfy

$$\frac{d}{dr}\left(r^2\frac{dA}{dr}\right)+\Big[K^2(r)\,r^2-\ell(\ell+1)\Big]A(r)=0,\quad \ell\in\mathbb{Z}_0^+. \tag{6.1.24}$$

As before, the equation for $A(r)$ does not involve m; hence, the scattering matrix components do not depend on m, and can be written as simply

$$s_{\ell m}\;=\;s_\ell. \tag{6.1.25}$$

For any given $V(r)$, we can solve the second-order ordinary differential equation numerically by supplying two boundary conditions at $r=0$, integrating up to a large value of r, and matching to the exterior solution

$$A(r)\;\stackrel{r\to\infty}{\longrightarrow}\;c_\ell^-\,h_\ell^-(kr)+c_\ell^+\,h_\ell^+(kr)=c_\ell^-\Big(h_\ell^-(kr)+s_\ell h_\ell^+(kr)\Big). \tag{6.1.26}$$

The value of s_ℓ can then be extracted.

To simplify the problem even further, let the scattering potential take the form of a spherical potential well of radius R and depth U:

$$V(r)=\begin{cases}-U & \text{for }\;r<R,\\ 0 & \text{otherwise.}\end{cases} \tag{6.1.27}$$

We will take $U>0$, so that the potential is attractive. (The interested reader can work through the repulsive case, $U<0$. The process is almost the same as what is presented below, except that for some values of E, the wave inside the scatterer becomes evanescent.) Now, the Schrödinger wave equation in the interior region reduces to the Helmholtz equation, but with k replaced with

$$q=\sqrt{2m(E+U)/\hbar^2}. \tag{6.1.28}$$

Note that $q\in\mathbb{R}^+$ for $E>0$, since we have assumed that $U>0$. The elementary solutions for $A(r)$ in the interior region are $j_\ell(qr)$ and $y_\ell(qr)$. However, we must exclude the latter, since they diverge at $r=0$. (When we got to a similar point in Section A.1, we did not exclude the spherical Bessel functions of the second kind, because at the time we were concerned with solutions in the exterior region.) We thus arrive at a solution of the form

$$A(r)=\begin{cases}\alpha_\ell\,j_\ell(qr), & r\le R\\ c_\ell^-\Big(h_\ell^-(kr)+s_\ell h_\ell^+(kr)\Big) & r\ge R.\end{cases} \tag{6.1.29}$$

So far, the values of α_ℓ, c_ℓ^-, and s_ℓ remain unknown. To proceed, we match the wavefunction and its derivative at the boundary $r=R$:

$$\begin{aligned}\alpha_\ell\,j_\ell(qR)&=c_\ell^-\Big(h_\ell^-(kR)+s_\ell h_\ell^+(kR)\Big)\\ \alpha_\ell\,qj_\ell'(qR)&=c_\ell^-\,k\Big(h_\ell^{-\prime}(kR)+s_\ell h_\ell^{+\prime}(kR)\Big).\end{aligned} \tag{6.1.30}$$

Here, j_ℓ' denotes the derivative of the spherical Bessel function, and likewise for $h_\ell^{\pm\prime}$. Taking the ratio of these two equations eliminates α_ℓ and c_ℓ^-:

$$\frac{qj_\ell'(qR)}{j_\ell(qR)} = k\frac{h_\ell^{-\prime}(kR) + s_\ell h_\ell^{+\prime}(kR)}{h_\ell^-(kR) + s_\ell h_\ell^+(kR)}. \tag{6.1.31}$$

With a bit of rearrangement, this becomes

$$s_\ell = -\frac{kh_\ell^{-\prime}(kR)j_\ell(qR) - qh_\ell^-(kR)j_\ell'(qR)}{kh_\ell^{+\prime}(kR)j_\ell(qR) - qh_\ell^+(kR)j_\ell'(qR)}. \tag{6.1.32}$$

The numerator and denominator are complex conjugates of one another, since j_ℓ is real and $(h_\ell^+)^* = h_\ell^-$. Hence,

$$s_\ell = e^{2i\delta_\ell}, \quad \text{where} \;\; \delta_\ell = \frac{\pi}{2} - \arg\left[kh_\ell^{+\prime}(kR)j_\ell(qR) - qh_\ell^+(kR)j_\ell'(qR)\right]. \tag{6.1.33}$$

In other words, the scattering matrix component is a pure phase factor. This is actually a consequence of energy conservation. Since the scattering matrix does not couple different angular momentum channels (due to the spherical symmetry), the incoming flux and outgoing flux in each channel must be equal. Hence, the only thing the scattering potential can do is to shift the phase of the outgoing spherical wave component in each channel.

Once we find δ_ℓ, we can compute the scattering amplitude

$$f(\mathbf{k}_i \to k\hat{\mathbf{r}}) = \frac{2\pi}{ik}\sum_{\ell=0}^{\infty}\left(e^{2i\delta_\ell} - 1\right)\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}). \tag{6.1.34}$$

This can be simplified with the aid of the following addition theorem for spherical harmonics:

$$P_\ell(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\mathbf{r}}_1)Y_{\ell m}(\hat{\mathbf{r}}_2). \tag{6.1.35}$$

where $P_\ell(\cdots)$ denotes a Legendre polynomial. We finally obtain

Definition: Legendre Polynomial

$$\begin{aligned} f(\mathbf{k}_i \to k\hat{\mathbf{r}}) &= \frac{1}{2ik}\sum_{\ell=0}^{\infty}\left(e^{2i\delta_\ell} - 1\right)\left(2\ell+1\right)P_\ell(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}}) \\ \delta_\ell &= \frac{\pi}{2} - \arg\left[kh_\ell^{+\prime}(kR)\, j_\ell(qR) - qh_\ell^+(kR)\, j_\ell'(qR)\right] \\ k &= |\mathbf{k}_i| = \sqrt{2mE/\hbar^2}, \;\; q = \sqrt{2m(E+U)/\hbar^2}. \end{aligned} \tag{6.1.36}$$

This result for the scattering amplitude depends upon two variables: (i) E, the particle energy (which is conserved), and (ii) $\Delta\theta = \cos^{-1}(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}})$, the **deflection angle** (i.e., the angle between the direction of incidence and the direction into which the particle is scattered).

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6.2: B- The Transfer Matrix Method

The **transfer matrix method** is a numerical method for solving the 1D Schrödinger equation, and other similar equations. In this method, the wavefunction at each point is decomposed into two complex numbers, called wave components. The wave components at any two points are related by a complex 2×2 matrix, called the **transfer matrix**.

B.1 Wave Components in 1D

For a 1D space with spatial coordinates x, the Schrödinger wave equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{6.2.1}$$

where m is the particle mass, $\psi(x)$ is the wavefunction, $V(x)$ is the potential function, and E is the energy. We treat E as an adjustable parameter (e.g., the energy of the incident particle in a scattering experiment).

Within any region of space where V is constant, the Schrödinger equation reduces to a 1D Helmholtz equation, whose general solution is

$$\psi(x) = A\,e^{ikx} + B\,e^{-ikx}, \quad \text{where} \quad k = \sqrt{\frac{2m[E-V(x)]}{\hbar^2}}. \tag{6.2.2}$$

If $E > V$, then the wave-number k is real and positive, and $\exp(\pm ikx)$ denotes a right-moving $(+)$ or left-moving $(-)$ wave. If $E < V$, then k is purely imaginary, and we choose the branch of the square root so that it is a positive multiple of i, so that $\exp(\pm ikx)$ denotes a wave that *decreases* exponentially toward the right $(+)$ or toward the left $(-)$.

We can re-write the two terms on the right-hand side as

$$\psi(x) = \psi_+(x) + \psi_-(x). \tag{6.2.3}$$

At each position x, the complex quantities $\psi_\pm(x)$ are called the **wave components** .

The problem statement for the transfer matrix method is as follows. Suppose we have a **piecewise-constant potential function** $V(x)$, which takes on values $\{V_1, V_2, V_3, \ldots\}$ in different regions of space, as shown in the figure below:

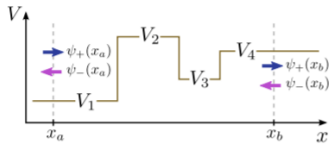

Figure 6.2.1

Given the wave components $\{\psi_+(x_a), \psi_-(x_a)\}$ at one position x_a, we seek to compute the wave components $\{\psi_+(x_b), \psi_-(x_b)\}$ at another position x_b. In general, these are related by a linear relation

$$\Psi_b = \mathbf{M}(x_b, x_a)\,\Psi_a, \tag{6.2.4}$$

where

$$\Psi_b = \begin{bmatrix}\psi_+(x_b)\\ \psi_-(x_b)\end{bmatrix}, \quad \Psi_a = \begin{bmatrix}\psi_+(x_a)\\ \psi_-(x_a)\end{bmatrix}. \tag{6.2.5}$$

The 2×2 matrix $\mathbf{M}(x_b, x_a)$ is called a **transfer matrix**. Take note of the notation in the parentheses: we put the "start point" x_a in the right-hand input, and the "end point" x_b in the left-hand input. We want to find $\mathbf{M}(x_b, x_a)$ from the potential and the energy E.

B.2 Constructing the Transfer Matrix

Consider the simplest possible case, where the potential has a single constant value V everywhere between two positions x_a and x_b, with $x_b > x_a$. Then, as we have just discussed, the solution throughout this region takes the form

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where} \quad k = \sqrt{\frac{2m(E-V)}{\hbar^2}}, \tag{6.2.6}$$

for some $A, B \in \mathbb{C}$. The wave components at the two positions are

$$\Psi_a = \begin{bmatrix}Ae^{ikx_a}\\ Be^{ikx_a}\end{bmatrix}, \quad \Psi_b = \begin{bmatrix}Ae^{ikx_b}\\ Be^{ikx_b}\end{bmatrix}. \tag{6.2.7}$$

Each component of Ψ_b is $\exp[ik(x_b - x_a)]$ times the corresponding component of Ψ_a. We can therefore eliminate A and B, and write

$$\Psi_b = \mathbf{M}_0(k, x_b - x_a)\Psi_a, \quad \text{where} \quad \mathbf{M}_0(k, L) \equiv \begin{bmatrix}e^{ikL} & 0\\ 0 & e^{-ikL}\end{bmatrix}. \tag{6.2.8}$$

The 2×2 matrix $\mathbf{M}_0(k, L)$ is the transfer matrix across a segment of constant potential. Its first input is the wave-number within the segment (determined by the energy E and potential V), and its second input is the segment length.

Next, consider a potential step at some position x_0, as shown in the figure below:

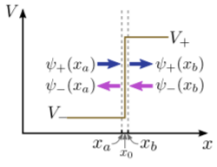

Figure 6.2.2

Let x_a and x_b be two points that are infinitesimally close to the potential step on either side (i.e., $x_a = x_0 - 0^+$ and $x_b = x_0 + 0^+$, where 0^+ denotes a positive infinitesimal). To the left of the step, the potential is V_-; to the right, the potential is V_+. The corresponding wave-numbers are

$$k_\pm = \sqrt{\frac{2m(E-V_\pm)}{\hbar^2}} \tag{6.2.9}$$

There are two important relations between the wavefunctions on the two sides of the step. Firstly, any quantum mechanical wavefunction must be continuous everywhere (otherwise, the Schrödinger equation would not be well-defined); this includes the point x_0, so

$$\psi_+(x_a) + \psi_-(x_a) = \psi_+(x_b) + \psi_-(x_b). \tag{6.2.10}$$

Secondly, since the potential is non-singular at x_0 the derivative of the wavefunction should be continuous at that point (this can be shown formally by integrating the Schrödinger across an infinitesimal interval around x_0). Hence,

$$ik_- \left[\psi_+(x_a) - \psi_-(x_a)\right] = ik_+ \left[\psi_+(x_b) - \psi_-(x_b)\right]. \tag{6.2.11}$$

These two equations can be combined into a single matrix equation:

$$\begin{bmatrix} 1 & 1 \\ k_- & -k_- \end{bmatrix} \begin{bmatrix} \psi_+(x_a) \\ \psi_-(x_a) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ k_+ & -k_+ \end{bmatrix} \begin{bmatrix} \psi_+(x_b) \\ \psi_-(x_b) \end{bmatrix}. \tag{6.2.12}$$

After doing a matrix inversion, this becomes

$$\Psi_b = \mathbf{M}_s(k_+, k_-)\, \Psi_a, \quad \text{where} \quad \mathbf{M}_s(k_+, k_-) = \frac{1}{2}\begin{bmatrix} 1+\frac{k_-}{k_+} & 1-\frac{k_-}{k_+} \\ 1-\frac{k_-}{k_+} & 1+\frac{k_-}{k_+} \end{bmatrix}. \tag{6.2.13}$$

The 2×2 matrix $\mathbf{M}_s(k_+, k_-)$ is the transfer matrix to go rightward from a region of wave-number k_-, to a region of wave-number k_+. Note that when $k_- = k_+$, this reduces to the identity matrix, as expected.

Using the above results, we can find the transfer matrix for any piecewise-constant potential. Consider the potential function shown below. It consists of segments of length $L_1, L_2, \ldots L_N$, with potential $V_1, V_2, \ldots, V_N$; outside, the potential is V_0:

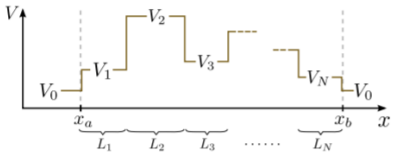

Figure 6.2.3

Let x_a and x_b lie right beyond the first and last segments (where $V = V_0$), with $x_b > x_a$. We can compute Ψ_b by starting with Ψ_a, and left-multiplying by a sequence of transfer matrices, one after the other. These transfer matrices consist of the two types derived in the previous sections: $\mathbf{M}_0$ (to cross a uniform segment) and $\mathbf{M}_s$ (to cross a potential step). Each matrix multiplication "transfers" us to another point to the right, until we reach x_b.

The overall transfer matrix between the two points is

Definition: Transfer Matrix

$$\begin{aligned} \mathbf{M}(x_b, x_a) &= \mathbf{M}_s(k_0, k_N)\, \mathbf{M}_0(k_N, L_N)\, \mathbf{M}_s(k_N, k_{N-1}) \cdots \\ &\quad \cdots \mathbf{M}_0(k_2, L_2)\, \mathbf{M}_s(k_2, k_1)\, \mathbf{M}_0(k_1, L_1)\, \mathbf{M}_s(k_1, k_0) \\ \text{where} \quad \mathbf{M}_0(k, L) &= \begin{bmatrix} e^{ikL} & 0 \\ 0 & e^{-ikL} \end{bmatrix} \\ \mathbf{M}_s(k_+, k_-) &= \frac{1}{2}\begin{bmatrix} 1+\frac{k_-}{k_+} & 1-\frac{k_-}{k_+} \\ 1-\frac{k_-}{k_+} & 1+\frac{k_-}{k_+} \end{bmatrix} \\ k_n &= \sqrt{\frac{2m(E-V_n)}{\hbar^2}}. \end{aligned} \tag{6.2.14}$$

The expression for $\mathbf{M}(x_b, x_a)$ should be read from right to left. Starting from x_a, we cross the potential step into segment 1, then pass through segment 1, cross the potential step from segment 1 to segment 2, pass through segment 2, and so forth. (Note that as we move left-to-right through the structure, the matrices are assembled right-to-left; a common mistake when writing a program to implement the transfer matrix method is to assemble the matrices in the wrong order, i.e. right-multiplying instead of left-multiplying.)

B.3 Reflection and Transmission Coefficients

The transfer matrix method is typically used to study how a 1D potential scatters an incident wave. Consider a 1D scatterer that is confined within a region $x_a \le x \le x_b$:

$$V(x) = 0 \quad \text{for} \quad x < x_a \text{ or } x > x_b. \tag{6.2.15}$$

The total wavefunction consists of an incident wave and a scattered wave,

$$\psi(x) = \psi_i(x) + \psi_s(x). \tag{6.2.16}$$

The incident wave is assumed to be incident from the left:

$$\psi_i(x) = \Psi_i\, \exp[ik_0(x - x_a)], \quad \text{where} \quad k_0 = \sqrt{\frac{2mE}{\hbar^2}}. \tag{6.2.17}$$

We have inserted the extra phase factor of $\exp(-ik_0 x_a)$ to ensure that $\psi_i(x_a) = \Psi_i$, which will be convenient. The wave is scattered as it meets the structure, and part of it is reflected back to the left, while another part is transmitted across to the right. Due to the linearity of the Schrödinger wave equation, the total wavefunction must be directly proportional to Ψ_i. Let us write the wave components at x_z and x_b as

$$\Psi(x_a) = \begin{bmatrix} \psi_+(x_a) \\ \psi_-(x_a) \end{bmatrix} = \Psi_i \begin{bmatrix} 1 \\ r \end{bmatrix} \tag{6.2.18}$$

$$\Psi(x_b) = \begin{bmatrix} \psi_+(x_b) \\ \psi_-(x_b) \end{bmatrix} = \Psi_i \begin{bmatrix} t \\ 0 \end{bmatrix}. \tag{6.2.19}$$

The complex numbers r and t are called the **reflection coefficient** and the **transmission coefficient**, respectively. Their values do *not* depend on Ψ_i, since they specify the wave components for the reflected and transmitted waves *relative* to Ψ_i. Note also that there is no ψ_- wave component at x_b, as the scattered wavefunction must be purely outgoing.

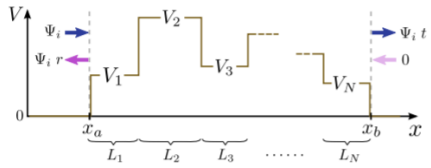

Figure 6.2.4

From the reflection and transmisison coefficients, we can also define the real quantities

$$R = |r|^2, \quad T = |t|^2, \tag{6.2.20}$$

which are called the **reflectance** and **transmittance** respectively. These are directly proportional to the total current flowing to the left and right.

According to the transfer matrix relation,

$$\begin{bmatrix} t \\ 0 \end{bmatrix} = \mathbf{M}(x_b, x_a) \begin{bmatrix} 1 \\ r \end{bmatrix}. \tag{6.2.21}$$

Hence, r and t can be expressed in terms of the components of the transfer matrix:

$$r = \frac{M_{21}}{M_{22}}, \quad t = \frac{M_{11}M_{22} - M_{12}M_{21}}{M_{22}} = \frac{\det(\mathbf{M})}{M_{22}}. \tag{6.2.22}$$

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6.3: C- Entropy

"Entropy" is a concept used in multiple fields of science and mathematics to quantify one's lack of knowledge about a complex system. In physics, its most commonly-encountered form is **thermodynamic entropy**, which describes the uncertainty about the microscopic configuration, or "microstate", of a large physical system. In the field of mathematics known as information theory, **information entropy** (also called **Shannon entropy** after its inventor C. Shannon) describes the uncertainty about the contents of a transmitted message. One of the most profound developments in theoretical physics in the 20th century was the discovery by E. T. Jaynes that statistical mechanics can be formulated in terms of information theory; hence, the thermodynamics-based and information-based concepts of entropy are one and the same. For details about this connection, see Jaynes (1957) and Jaynes (1957a). This appendix summarizes the definition of entropy in classical physics, and how it is related to other physical quantities.

C.1 Definition

Suppose a system has W discrete microstates labeled by integers $\{1, 2, 3, \ldots, W\}$ These microstates are associated with probabilities $\{p_1, p_2, p_3, \ldots, p_W\}$, subject to the conservation of total probability

$$\sum_{i=1}^{W} p_i = 1. \tag{6.3.1}$$

We will discuss how these microstate probabilities are chosen later (see Section 3). Given a set of these probabilities, the entropy is defined as

$$S = -k_b \sum_{i=1}^{W} p_i \ln(p_i). \tag{6.3.2}$$

Here, k_b is Boltzmann's constant, which gives the entropy units of $[E/T]$ (energy per unit temperature); this is a remnant of entropy's origins in 19th century thermodynamics, and is omitted by mathematicians.

It is probably not immediately obvious why Equation (6.3.2) is useful. To understand it better, consider its behavior under two extreme scenarios:

- Suppose the microstate is definitely known, i.e., $p_k = 1$ for some k. Then $S = 0$.
- Suppose there are W possible microstates, each with equal probabilities

$$p_i = \frac{1}{W} \quad \forall i \in \{1, 2, \ldots, W\}. \tag{6.3.3}$$

  This describes a scenario of complete uncertainty between the possible choices. Then

$$S = -k_b W \frac{1}{W} \ln(1/W) = k_b \ln W. \tag{6.3.4}$$

The entropy formula is designed so that any other probability distribution—i.e., any situation of *partial* uncertainty—yields an entropy S between 0 and $k_b \ln W$.

To see that zero is the lower bound for the entropy, note that for $0 \leq p_i \leq 1$, each term in the entropy formula (6.3.2) satisfies $-k_b\, p_i \ln(p_i) \geq 0$, and the equality holds if and only if $p_i = 0$ or $p_i = 1$. This is illustrated in the figure below:

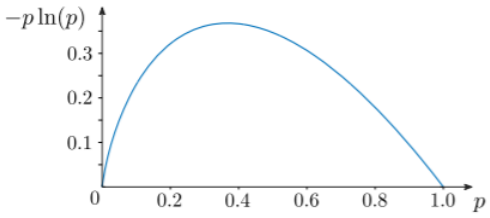

Figure 6.3.1

This implies that $S \geq 0$. Moreover, $S = 0$ if and only if $p_i = \delta_{ik}$ for some k (i.e., there is no uncertainty about which microstate the system is in).

Next, it can be shown that S is bounded above by $k_b \ln W$, a relation known as Gibbs' inequality. This follows from the fact that $\ln x \leq x - 1$ for all positive x, with the equality occurring if and only if $x = 1$. Take $x = 1/(Wp_i)$ where W is the number of microstates:

$$\begin{aligned} \ln\left[\frac{1}{Wp_i}\right] &\leq \frac{1}{Wp_i} - 1 \quad \text{for all } i = 1, \ldots, W. \\ \sum_{i=1}^{W} p_i \ln\left[\frac{1}{Wp_i}\right] &\leq \sum_{i=1}^{W} \left(\frac{1}{W} - p_i\right) \\ -\sum_{i=1}^{W} p_i \ln W - \sum_{i=1}^{W} p_i \ln p_i &\leq 1 - 1 = 0 \\ -k_b \sum_{i=1}^{W} p_i \ln p_i &\leq k_b \ln W. \end{aligned} \tag{6.3.5}$$

Moreover, the equality holds if and only if $p_i = 1/W$ for all i.

C.2 Extensivity

Another important feature of the entropy is that it is **extensive**, meaning that it scales proportionally with the size of the system. Consider two independent systems A and B, which have microstate probabilities $\{p_i^A\}$ and $\{p_j^B\}$. If we treat the combination of A and B as a single system, each microstate of the combined system is specified by one microstate of A and one of B, with probability $p_{ij} = p_i^A p_j^B$. The entropy of the combined system is

$$\begin{aligned} S &= -k_b \sum_{ij} p_i^A p_j^B \ln\left(p_i^A p_j^B\right) \\ &= -k_b \Big(\sum_i p_i^A \ln p_i^A\Big)\Big(\sum_j p_j^B\Big) - k_b \Big(\sum_i p_i^A\Big)\Big(\sum_j p_j^B \ln p_j^B\Big) \\ &= S_A + S_B, \end{aligned} \tag{6.3.6}$$

where S_A and S_B are the individual entropies of the A and B subsystems.

C.3 Entropy and Thermodynamics

The theory of statistical mechanics seeks to describe the macroscopic behavior of a large physical system by assigning some set of probabilities $\{p_1, p_2, \ldots, p_W\}$ to its microstates. How are these probabilities chosen? One elegant way is to use the following postulate:

Postualte 6.3.1

Choose $\{p_1, \ldots, p_W\}$ so as to maximize S, subject to constraints imposed by known facts about the macroscopic state of the system.

The idea is that we want a probability distribution that is as "neutral" as possible, while being consistent with the available macroscopic information about the system.

For instance, suppose the only information we have about the macroscopic state of the system is that its energy is precisely E. In this scenario, called a **micro-canonical ensemble**, we maximize S by assigning equal probability to every microstate of energy E, and zero probability to all other microstates, for reasons discussed in Section 1. (In some other formulations of statistical mechanics, this assignment of equal probabilities is treated as a postulate, called the **ergodic hypothesis**.)

Or suppose that only the system's *mean* energy $\langle E \rangle$ is known, and nothing else. In this case, we can maximize S using the method of Lagrange multipliers. The relevant constraints are the given value of $\langle E \rangle$ and conservation of probability:

$$\langle E \rangle = \sum_i E_i \, p_i, \quad \sum_i p_i = 1. \tag{6.3.7}$$

We thus introduce two Lagrange multiplers, λ_1 and λ_2. For every microstate i, we require

$$\begin{aligned} \frac{\partial S}{\partial p_i} + \lambda_1 \frac{\partial}{\partial p_i}\left(\sum_j E_j p_j\right) + \lambda_2 \frac{\partial}{\partial p_i}\left(\sum_j p_j\right) &= 0 \\ \Rightarrow \quad -k_b\left(\ln p_i + 1\right) + \lambda_1 E_i + \lambda_2 &= 0. \end{aligned} \tag{6.3.8}$$

Upon taking $\lambda_1 = -1/T$ as the *definition* of the temperature T, we obtain the celebrated **Boltzmann distribution**:

$$p_i = \frac{e^{-E/k_b T}}{Z}, \quad \text{where} \quad Z = \sum_i e^{-E/k_b T}. \tag{6.3.9}$$

Further Reading

- E. T. Jaynes, *Information theory and statistical mechanics*, Physical Review **106**, 620 (1957).
- E. T. Jaynes, *Information theory and statistical mechanics. ii*, Physical Review **108**, 171 (1957).

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6.4: D- Numerical Tensor Products

This appendix discusses how tensor products are handled in numerical linear algebra software. We will focus on Python with the Numeric Python (numpy) module. The discussion is also applicable, with minor modifications, to GNU Octave or Matlab. We assume the reader is familiar with the basics of Python/Numpy, e.g. how vectors can be represented by 1D arrays, linear operators (matrices) can be represented by 2D arrays, etc.

Tensor products are implemented by the `numpy.kron` function, which performs an operation called a **Kronecker product**. The function takes two inputs, which can be 1D arrays, 2D arrays, or even higher-dimensional arrays (which we won't discuss). It returns a new array representing the tensor product of the inputs, whose dimensionality depends on that of the inputs. The function can be used to compute products of vectors ($|a\rangle \otimes |b\rangle$), products of operators ($\hat{O}_A \otimes \hat{O}_B$), etc. It can even compute "mixed" products like $|a\rangle \otimes \hat{O}_B$, which is useful for calculating partial projections and partial traces.

In the next few sections, we will prove that the various tensor products of bras, kets, and operators can be represented using the following Numpy expressions involving `numpy.kron`:

Definition: Numpy Expressions

$$
\begin{aligned}
|a\rangle \otimes |b\rangle &\leftrightarrow \texttt{kron(a, b)} & \langle a| \otimes \langle b| &\leftrightarrow \texttt{kron(a.conj(), b.conj())} \\
\hat{A} \otimes \hat{B} &\leftrightarrow \texttt{kron(A, B)} & & \\
|a\rangle \otimes \hat{B} &\leftrightarrow \texttt{kron(a, B.T).T} & \langle a| \otimes \hat{B} &\leftrightarrow \texttt{kron(a.conj(), B)} \\
\hat{A} \otimes |b\rangle &\leftrightarrow \texttt{kron(A.T, b).T} & \hat{A} \otimes \langle b| &\leftrightarrow \texttt{kron(A, b.conj())}
\end{aligned}
$$

D.1 Products of Vectors

Suppose a and b are both 1D arrays, of length M and N respectively; let their components be $(a_0, a_1, \ldots, a_{M-1})$ and $(b_0, b_1, \ldots, b_{N-1})$. Following Numpy conventions, we do not explicitly distinguish between "row vectors" and "column vectors", and component indices start from 0. The Kronecker product between a and b generates the following 1D array:

$$\texttt{kron}(a, b) = \Big(a_0 b_0,\ \ldots,\ a_0 b_{N-1},\ a_1 b_0,\ \ldots,\ a_1 b_{N-1},\ \ldots,\ a_{M-1} b_{N-1}\Big). \tag{6.4.1}$$

We can think of this as *taking each component of a, and multiplying it by the entire b array*:

$$\texttt{kron}(a, b) = \Big(a_0 b,\ a_1 b,\ \ldots,\ a_{M-1} b\Big). \tag{6.4.2}$$

As we shall see, this description of the Kronecker product extends to higher-dimensional arrays as well. In the present case, a and b are both 1D, and the result is a 1D array of MN components, which can be described compactly in index notation by

$$\big[\,\texttt{kron}(a, b)\,\big]_\mu = a_m\, b_n \quad \text{where} \quad \mu = mN + n. \tag{6.4.3}$$

The index μ is defined so that as we sweep through $m = 0, \ldots, M-1$ and $n = 0, \ldots, N-1$, μ runs through the values $0, 1, \ldots, MN-1$ without duplication. Note, by the way, that the order of inputs into `kron` is important: $\texttt{kron}(a, b)$ is not the same as $\texttt{kron}(b, a)$! The asymmetry between a and b is apparent in the definitions (6.4.1) and (6.4.2).

In terms of abstract linear algebra (as used in quantum theory), let $\mathscr{H}_A$ be an M-dimensional space with basis $\{|m\rangle\}$, and $\mathscr{H}_B$ be an N-dimensional space with basis $\{|n\rangle\}$. Any two vectors $|a\rangle \in \mathscr{H}_A$ and $|b\rangle \in \mathscr{H}_B$ can be written as

$$|a\rangle = \sum_{m=0}^{M-1} a_m |m\rangle, \quad |b\rangle = \sum_{n=0}^{N-1} b_n |n\rangle. \tag{6.4.4}$$

A natural basis for the product space $\mathscr{H}_A \otimes \mathscr{H}_B$ is

$$\Big\{|\mu\rangle \equiv |m\rangle|n\rangle\Big\} \quad \text{where} \begin{cases} \mu &= mN+n \\ m &= 0,1,\ldots,M-1 \\ n &= 0,1,\ldots,N-1. \end{cases} \tag{6.4.5}$$

Using Equation (6.4.3), we can show that

$$|a\rangle \otimes |b\rangle = \sum_{mn} a_m b_n |m\rangle|n\rangle = \sum_{\mu=0}^{MN-1} \big[\texttt{kron}(a,b)\big]_\mu \, |\mu\rangle. \tag{6.4.6}$$

Therefore, we need only remember that the tensor product of two kets is represented by

$$|a\rangle \otimes |b\rangle \quad \leftrightarrow \quad \texttt{kron}(a,b). \tag{6.4.7}$$

Likewise, for bras,

$$\langle a| \otimes \langle b| \quad \leftrightarrow \quad \texttt{kron}(a^*,b^*). \tag{6.4.8}$$

D.2 Products of Matrices

Let A and B be 2D arrays of size $M \times M$ and $N \times N$ respectively:

$$A = \begin{bmatrix} A_{00} & \cdots & A_{0,M-1} \\ \vdots & \ddots & \vdots \\ A_{M-1,0} & \cdots & A_{M-1,M-1} \end{bmatrix}, \quad B = \begin{bmatrix} B_{00} & \cdots & B_{0,N-1} \\ \vdots & \ddots & \vdots \\ B_{N-1,0} & \cdots & B_{N-1,N-1} \end{bmatrix}. \tag{6.4.9}$$

Then the Kronecker product of A and B is an $MN \times MN$ array of the form

$$\texttt{kron}(A,B) = \begin{bmatrix} A_{00}B & \cdots & A_{0,M-1}B \\ \vdots & \ddots & \vdots \\ A_{M-1,0}B & \cdots & A_{M-1,M-1}B \end{bmatrix}. \tag{6.4.10}$$

As before, this can be interpreted as taking each component of A, and multiplying it by B. The result can be written using index notation as

$$\big[\texttt{kron}(A,B)\big]_{\mu\mu'} = A_{mm'}B_{nn'} \quad \text{where} \quad \mu = mN+n, \;\; \mu' = m'N+n'. \tag{6.4.11}$$

In the language of abstract linear algebra, let $\mathscr{H}_A$ and $\mathscr{H}_B$ again be spaces with bases $\{|m\rangle\}$ and $\{|n\rangle\}$. Consider two linear operators $\hat{A}$ and $\hat{B}$ acting respectively on these spaces:

$$\hat{A} = \sum_{m,m'=0}^{M-1} |m\rangle A_{mm'} \langle m'|, \quad \hat{B} = \sum_{n,n'=0}^{N-1} |n\rangle B_{nn'} \langle n'|. \tag{6.4.12}$$

Then we can show using Equation (6.4.11) that

$$\hat{A} \otimes \hat{B} = \sum_{mm'nn'} |m\rangle|n\rangle \, A_{mm'} B_{nn'} \, \langle m'|\langle n'| \tag{6.4.13}$$

$$= \sum_{\mu,\mu'} |\mu\rangle \, \big[\texttt{kron}(A,B)\big]_{\mu\mu'} \, \langle \mu'|, \tag{6.4.14}$$

where $\big\{|\mu\rangle\big\}$ is the basis for $\mathscr{H}_A \otimes \mathscr{H}_B$ previously defined in Equation (6.4.5). Thus,

$$\hat{A} \otimes \hat{B} \quad \leftrightarrow \quad \texttt{kron}(A,B). \tag{6.4.15}$$

This result, like Equation (6.4.7), is nice because it means that we can relegate the handling of tensor product components entirely to the `kron` function. So long as we make a particular basis choice for the spaces $\mathscr{H}_A$ and $\mathscr{H}_B$, and keep to that choice,

`kron` will return the vector products and operator products expressed using an appropriate and natural basis for $\mathscr{H}_A \otimes \mathscr{H}_B$ [i.e., the basis defined in Equation (6.4.5)].

D.3 Mixed Products

For "mixed" products of operators with bras or kets, the representation using `kron` is more complicated, but only slightly. First, consider the 1D array a and 2D array B:

$$a = (a_0, \ldots, a_{M-1}), \quad B = \begin{bmatrix} B_{00} & \cdots & B_{0,N-1} \\ \vdots & \ddots & \vdots \\ B_{N-1,0} & \cdots & B_{N-1,N-1} \end{bmatrix}. \tag{6.4.16}$$

Then the Kronecker product between the two is

$$\texttt{kron}(a, B) = (a_0 B, a_1 B, \ldots, a_{M-1} B). \tag{6.4.17}$$

Note that a is explicitly treated as a row vector. In component terms,

$$\texttt{kron}(a,\ B)]_{n\mu'} = a_{m'} B_{nn'}, \quad \text{where} \quad \mu' = m'N + n'. \tag{6.4.18}$$

In linear algebraic terms, let

$$|a\rangle = \sum_m a_m |m\rangle, \quad \hat{B} = \sum_{nn'} |n\rangle B_{nn'} \langle n'|. \tag{6.4.19}$$

Then

$$|a\rangle \otimes \hat{B} = \sum_{\mu n'} |\mu\rangle\, a_m B_{nn'}\, \langle n'|, \qquad \mu = mN + n. \tag{6.4.20}$$

This does not quite match Equation (6.4.18)! The basic problem is that the Kronecker product treats a a row vector. However, we can patch things up by massaging Equation (6.4.18) a bit:

$$\begin{aligned} [\texttt{kron}(a, B^T)^T]_{\mu n'} &= [\texttt{kron}(a, B^T)]_{n'\mu} \\ &= a_m (B^T)_{n'n} \qquad \text{where} \quad \mu' = m'N + n' \\ &= a_m B_{nn'}. \end{aligned} \tag{6.4.21}$$

This is an appropriate match for Equation (6.4.20), so we conclude that

$$|a\rangle \otimes \hat{B} \quad \leftrightarrow \quad \texttt{kron}(a, B^T)^T. \tag{6.4.22}$$

To take the product using the bra $\langle a|$, we replace Equation (6.4.20) by

$$\langle a| \otimes \hat{B} = \sum_{n\mu'} |n\rangle\, a^*_{m'} B_{nn'}\, \langle \mu'|, \qquad \mu' = m'N + n'. \tag{6.4.23}$$

Comparing this to Equation (6.4.18) yields

$$\langle a| \otimes \hat{B} \quad \leftrightarrow \quad \texttt{kron}(a^*, B). \tag{6.4.24}$$

Likewise, consider the 2D array A and 1D array b:

$$A = \begin{bmatrix} A_{00} & \cdots & A_{0,M-1} \\ \vdots & \ddots & \vdots \\ A_{M-1,0} & \cdots & A_{M-1,M-1} \end{bmatrix}, \quad b = (b_0, \ldots, b_{N-1}). \tag{6.4.25}$$

Then the Kronecker product is

$$\texttt{kron}(A,b) = \begin{bmatrix} A_{00}b & \cdots & A_{0,M-1}b \\ \vdots & \ddots & \vdots \\ A_{M-1,0}b & \cdots & A_{M-1,M-1}b \end{bmatrix}. \tag{6.4.26}$$

Similar to before, b is treated as a row vector. In component terms,

$$[\texttt{kron}(A,\ B)]_{m\mu'} = A_{mm'}b_{n'}, \quad \text{where} \quad \mu' = m'N + n'. \tag{6.4.27}$$

Using the same procedure as before, we can straightforwardly show that

$$\hat{A} \otimes |b\rangle = \sum_{\mu m'} |\mu\rangle \, [\texttt{kron}(A^T, b)^T]_{\mu m'} \, \langle m'| \qquad \leftrightarrow \quad \texttt{kron}(A^T, b)^T \tag{6.4.28}$$

$$\hat{A} \otimes \langle b| = \sum_{m\mu'} |m\rangle \, [\texttt{kron}(A, b^*)]_{m\mu'} \, \langle \mu'| \qquad \leftrightarrow \quad \texttt{kron}(A, b^*). \tag{6.4.29}$$

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6.5: E- Coherent States

Coherent states are special states of bosonic systems (including the quantum harmonic oscillator, whose excitation quanta can be regarded as bosonic particles) whose dynamics are highly similar to classical oscillator trajectories. They provide an important link between quantum and classical harmonic oscillators.

E.1 Definition

The Hamiltonian of a simple harmonic oscillator (with $\hbar = m = \omega_0 = 1$ for simplicity) is

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}, \tag{6.5.1}$$

where $\hat{x}$ and $\hat{p}$ are the position and momentum operators. The ladder operators are

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \tag{6.5.2}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p})\,. \tag{6.5.3}$$

These obey the commutation relation

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{6.5.4}$$

As a result, we can also regard these as the creation and annihilation operators for a bosonic particle that has only one single-particle state.

The Hamiltonian for the harmonic oscillator, Equation (6.5.1), can be written as

$$\hat{H} = \hat{a}^\dagger \hat{a} + 1/2. \tag{6.5.5}$$

The annihilation operator $\hat{a}$ kills off the ground state $|\varnothing\rangle$:

$$\hat{a}|\varnothing\rangle = 0. \tag{6.5.6}$$

Thus, $|\varnothing\rangle$ is analogous to the "vacuum state" for a bosonic particle.

Returning to the Hamiltonian (6.5.1), suppose we add a term proportional to $\hat{x}$:

$$\hat{H}' = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} - \sqrt{2}\alpha_1 \hat{x}. \tag{6.5.7}$$

The coefficient of $-\sqrt{2}\alpha_1$, where $\alpha_1 \in \mathbb{R}$, is for later convenience. By completing the square, we see that this additional term corresponds to a shift in the center of the potential, plus an energy shift:

$$\hat{H}' = \frac{\hat{p}^2}{2} + \frac{1}{2}\left(\hat{x} - \sqrt{2}\alpha_1\right)^2 - \alpha_1^2. \tag{6.5.8}$$

Let $|\alpha_1\rangle$ denote the ground state for the shifted harmonic oscillator.

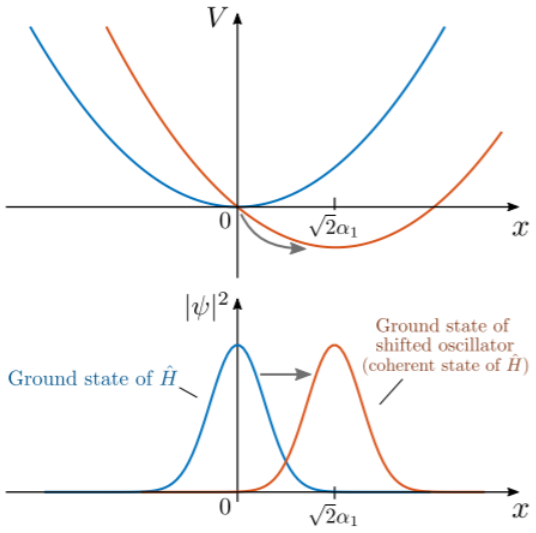

Figure 6.5.1

By analogy with how we solved the original harmonic oscillator problem, let us define a new annihilation operator with displaced x:

$$\hat{a}' = \frac{1}{\sqrt{2}}\left(\hat{x} - \sqrt{2}\alpha_1 + i\hat{p}\right). \tag{6.5.9}$$

This is related to the original annihilation operator by

$$\hat{a}' = \hat{a} - \alpha_1. \tag{6.5.10}$$

We can easily show that $[\hat{a}', \hat{a}'^{\dagger}] = 1$, and that $\hat{H}' = \hat{a}'^{\dagger}\hat{a}' + 1/2 - \alpha_1^2$. Hence,

$$\hat{a}'\,|\alpha_1\rangle = 0. \tag{6.5.11}$$

But Equation (6.5.10) implies that in terms of the *original* annihilation operator,

$$\hat{a}\,|\alpha_1\rangle = \alpha_1\,|\alpha_1\rangle. \tag{6.5.12}$$

In other words, $|\alpha_1\rangle$ is an eigenstate of the original harmonic oscillator's annihilation operator, with the displacement parameter α_1 as the corresponding eigenvalue! For reasons that will become clear later, we call $|\alpha_1\rangle$ a **coherent state** of the original harmonic oscillator $\hat{H}$.

E.2 Explicit Expression for the Coherent State

Let us derive an explicit expression for the coherent state in terms of $\hat{a}$ and $\hat{a}^{\dagger}$, the creation and annihilation operators of the original harmonic oscillator. Consider the translation operator

$$\hat{T}(\Delta x) = \exp(-i\hat{p}\Delta x). \tag{6.5.13}$$

Since $|\alpha_1\rangle$ is the ground state of a displaced harmonic oscillator, it can be generated by performing a displacement of the original oscillator's ground state $|\varnothing\rangle$. The displacement is $\Delta x = \sqrt{2}\alpha_1$:

$$|\alpha_1\rangle = \hat{T}\left(\sqrt{2}\alpha_1\right)\,|\varnothing\rangle \tag{6.5.14}$$

$$= \exp\left[\alpha_1\left(\hat{a}^{\dagger} - \hat{a}\right)\right]|\varnothing\rangle. \tag{6.5.15}$$

In deriving the second line, we have used Equations (6.5.2)–(6.5.3) to express $\hat{p}$ in terms of $\hat{a}$ and $\hat{a}^{\dagger}$. We can further simplify the result by using the Baker-Campbell-Hausdorff formula for operator exponentials:

$$\text{If}\ \ [[\hat{A},\hat{B}],\hat{A}] = [[\hat{A},\hat{B}],\hat{B}] = 0 \ \ \Rightarrow\ \ e^{\hat{A}+\hat{B}} = e^{-[\hat{A},\hat{B}]/2}e^{\hat{A}}e^{\hat{B}}. \tag{6.5.16}$$

The result is

$$|\alpha_1\rangle = e^{-\alpha_1^2/2}\, e^{\alpha_1 \hat{a}^\dagger} |\varnothing\rangle. \tag{6.5.17}$$

If we write the exponential in its series form,

$$|\alpha_1\rangle = e^{-\alpha_1^2/2} \left(1 + \alpha_1 \hat{a}^\dagger + \frac{\alpha_1^2}{2}\left(\hat{a}^\dagger\right)^2 + \cdots\right) |\varnothing\rangle, \tag{6.5.18}$$

then we see that from the point of view of the bosonic excitations of the original Hamiltonian $\hat{H}$, the state $|\alpha_1\rangle$ has an *indeterminate number of bosons*. It is a superposition of the zero-boson (vacuum) state, a one-boson state, a two-boson state, etc.

We can generalize the coherent state by performing a shift not just in space, but also in momentum. Instead of Equation (6.5.7), let us define

$$\hat{H}' = \frac{1}{2}\left(\hat{p} - \sqrt{2}\alpha_2\right)^2 + \frac{1}{2}\left(\hat{x} - \sqrt{2}\alpha_1\right)^2 \tag{6.5.19}$$

$$= \hat{H} - \left(\alpha \hat{a}^\dagger + \alpha^* \hat{a}\right) + \text{constant}, \tag{6.5.20}$$

where

$$\alpha \equiv \alpha_1 + i\alpha_2 \ \in \ \mathbb{C}. \tag{6.5.21}$$

It can then be shown that the ground state of $\hat{H}'$, which we denote by $|\alpha\rangle$, satisfies

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle. \tag{6.5.22}$$

(Note that $\hat{a}$ is not Hermitian, so its eigenvalue α need not be real.) In explicit terms,

$$|\alpha\rangle \ = \ \exp\left[\alpha \hat{a}^\dagger - \alpha^* \hat{a}\right] |\varnothing\rangle \ = \ e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |\varnothing\rangle. \tag{6.5.23}$$

E.3 Basic Properties

There is one coherent state $|\alpha\rangle$ for each complex number $\alpha \in \mathbb{C}$. They have the following properties:

1. They are normalized:

   $$\langle\alpha|\alpha\rangle = 1. \tag{6.5.24}$$

   This follows from the fact that they are ground states of displaced harmonic oscillators.

2. They form a complete set, meaning that the identity operator can be resolved as

   $$\hat{I} = C \int d^2\alpha |\alpha\rangle\langle\alpha|, \tag{6.5.25}$$

   where C is some numerical constant and $\int d^2\alpha$ denotes an integral over the complex plane. However, the coherent states do *not* form an orthonormal set, as they are over-complete: $\langle\alpha|\alpha'\rangle \neq 0$ for $\alpha \neq \alpha'$.

3. The expected number of particles in a coherent state is

   $$\langle\alpha|\hat{a}^\dagger \hat{a}|\alpha\rangle = |\alpha|^2. \tag{6.5.26}$$

4. The probability distribution of the number of particles follows a *Poisson distribution*:

   $$P(n) = |\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!}. \tag{6.5.27}$$

   The mean and variance of this distribution are both $|\alpha|^2$.

5. The mean position and momentum are

   $$\langle\alpha|\hat{x}|\alpha\rangle = \sqrt{2}\,\mathrm{Re}(\alpha) \tag{6.5.28}$$

   $$\langle\alpha|\hat{p}|\alpha\rangle = \sqrt{2}\,\mathrm{Im}(\alpha). \tag{6.5.29}$$

E.4 Dynamical Properties

Take the harmonic oscillator Hamiltonian with zero-point energy omitted for convenience:

$$\hat{H} = \hat{a}^\dagger \hat{a}. \tag{6.5.30}$$

Suppose we initialize the system in a coherent state $|\alpha_0\rangle$ for some $\alpha_0 \in \mathbb{C}$. This is not an energy eigenstate of $\hat{H}$, so how will it subsequently evolve?

It turns out that the dynamical state has the form

$$|\psi(t)\rangle = |\alpha(t)\rangle, \quad \text{where} \;\; \alpha(0) = \alpha_0. \tag{6.5.31}$$

In other words, the system is always in a coherent state, but the complex parameter $\alpha(t)$ varies with time. To find $\alpha(t)$, plug the ansatz into the time-dependent Schrödinger equation:

$$i\frac{d}{dt}|\alpha(t)\rangle = \hat{a}^\dagger \hat{a}|\alpha(t)\rangle \tag{6.5.32}$$

$$i\left\langle \alpha(t)\right|\frac{d}{dt}\left|\alpha(t)\right\rangle = |\alpha(t)|^2. \tag{6.5.33}$$

We can calculate the left-hand side using Equations (6.5.22), (6.5.23), and (6.5.24):

$$i\left\langle \alpha(t)\right|\frac{d}{dt}\left|\alpha(t)\right\rangle = i\left\langle \alpha(t)\right| \frac{d}{dt}\exp\left[e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}\right]|\varnothing\rangle \tag{6.5.34}$$

$$= i\left\langle \alpha(t)\right| \left(-\frac{1}{2}\frac{d}{dt}(\alpha\alpha^*) + \frac{d\alpha}{dt}\hat{a}^\dagger\right)|\alpha(t)\rangle \tag{6.5.35}$$

$$= i\left(-\frac{1}{2}\dot{\alpha}\alpha^* - \frac{1}{2}\alpha\dot{\alpha}^* + \dot{\alpha}\alpha^*\right). \tag{6.5.36}$$

Hence,

$$\frac{i}{2}(\dot{\alpha}\alpha^* - \alpha\dot{\alpha}^*) = |\alpha|^2. \tag{6.5.37}$$

This looks more complicated than it actually is. Dividing both sides by $\alpha\alpha^*$ gives

$$\frac{1}{2}\left(\frac{i\dot{\alpha}}{\alpha} + \left[\frac{i\dot{\alpha}}{\alpha}\right]^*\right) = \mathrm{Re}\left[\frac{i\dot{\alpha}}{\alpha}\right] = 1. \tag{6.5.38}$$

This reduces to

$$\dot{\alpha} = \big[-i + \gamma(t)\big]\alpha(t), \quad \gamma \in \mathbb{R}. \tag{6.5.39}$$

This is the equation for a complex harmonic oscillator with an arbitrary damping or amplification factor γ. For $\gamma = 0$, the oscillator is energy-conserving and the solutions are

$$\alpha(t) = \alpha_0\, e^{-it}. \tag{6.5.40}$$

Referring back to Equations (6.5.28)–(6.5.29), this implies that the mean position and momentum have the following time-dependence:

$$\langle x\rangle = \;\; \sqrt{2}|\alpha_0|\cos[t - \arg(\alpha_0)] \tag{6.5.41}$$

$$\langle p\rangle = -\sqrt{2}|\alpha_0|\sin[t - \arg(\alpha_0)]. \tag{6.5.42}$$

The dynamics of a coherent state therefore reproduces the motion of a classical harmonic oscillator with $m = \omega_0 = 1$.

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